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MODEL PREDICTIVE CONTROL
OF
A SUSPENSION BATCH PVC REACTOR

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in Partial Fulfillment of the Requirements

for the Degree of

Master of Technology

by

Brajesh Kumar Singh

to the

**DEPARTMENT OF
CHEMICAL ENGINEERING
INDIAN INSTITUTE OF TECHNOLOGY, KANPUR**

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CERTIFICATE

It is certified that the work contained in this thesis entitled **Model Predictive Control of a Suspension Batch PVC Reactor** by *Brajesh Kumar Singh* has been carried out under my supervision and that this work has not been submitted elsewhere for a degree.

.....

(Dr. Ashok Khanna)

Assoc. Professor

Dept. of Chemical Engg.

IIT Kanpur - 208 006

INDIA

April, 1997

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Brajesh Kumar Singh

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IIT Kanpur.

Abstract

In the competitive atmosphere of today, batch chemical reactors are pinpointed as where better performance can be obtained through better process control. Recent advances in computer technology have made the implementation of modern control algorithms a possibility in industrial environments. Most of the chemical processes are nonlinear and difficult to model, so traditional linear controllers often fail to control nonlinear processes. With tighter constraints on product quality, environmental regulations and energy utilization, there is now a growing need for reliable predictive models and new on-line control algorithms for nonlinear processes.

In this work a Model Predictive Controller (MPC) is applied at the simulation level to a non-linear and time varying process of PVC batch reactor. We develop the linear model of the process by identification of the data (input-output information) and apply the MPC to control the temperature of the reactor, and molecular weight of the PVC. From different simulation results we discuss the performance of MPC under different cases (deterministic, stochastic-without filtering, and stochastic-with filtering). We also apply MPC in its adaptive form AMPC, by doing the on-line identification of the process and try to show from the different simulation runs that AMPC performs better in certain cases.

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Chapter 1

Introduction

1.1 General

PVC has been produced and processed in large volumes for a long time on account of its versatile properties in relation to its low price. The commercial production of PVC is based on three main processes: suspension, emulsion, and mass polymerization. The suspension process is presently the dominating route to PVC. A significant step in promoting the growth of PVC industry was the development of oxychlorination process which made it possible to use ethylene as feed stock for Vinyl Chloride Monomer (VCM) production. Another major factor for the growth of PVC industry is that it is the largest consumer of chlorine, which is essentially a by-product in the manufacture of sodium hydroxide. Currently next to polyethylene, PVC is the most frequently used thermoplastic material.

1.1.1 Polymerization

Polymerization of VCM is a free radical type of chain reaction. Suspension polymerization of VCM is carried out batchwise, mostly in stainless steel reactors having polished internal surfaces and sizes upto 200 m³. Continuous operation has not proven feasible. An important reason for this is that the residence time distribution has to be very narrow in order to avoid the formation of compact, hard-melting grains.

In suspension polymerization, liquid monomer (100 parts) is emulsified in water (150-200 parts). The emulsion is stabilized by small amounts of surface-active polymers, often in combination with a low molecular weight emulsifier. Polymerization is carried out using one or multiple monomer-soluble initiators. The stirring requirements are stringent. The reactors are jacketed and cooled through the reactor wall.

1.1.2 Physics

At normal temperatures, VCM is a gas. Its boiling temperature at normal pressure is -13.8°C and density is 890 kg/m^3 . The density of technical PVC falls into the range $1390\text{--}1400\text{ kg/m}^3$. The large difference between the densities of the monomer and its polymer implies that the volume decrease during polymerization is rather large.

PVC is insoluble in its monomer. From mass polymerization studies, Boisel and Fischer (1977) found that the solubility of the polymer formed at the start of the polymerization was lower than $10^{-3}\%$.

1.1.3 Chemistry and Kinetics

Commercially, all PVC is prepared by free-radical polymerization. The kinetics of vinyl chloride polymerization is to a large extent independent of the particular reaction conditions used, that is, whether mass, suspension, or emulsion processes are concerned. In all types of processes, the majority of the polymer is formed by reaction in a monomer swollen polymer phase, the composition of which is determined by the swelling equilibrium of the VCM/PVC system and, hence, does not depend on process type. Another important factor is the unusually high frequency of chain transfer to the monomer. The importance of this reaction explains why the molecular weight is determined by reaction temperature and is almost independent of the rate of initiation

and conversion. It also explains the fact that the MWD of PVC prepared under isothermal conditions closely approaches the most probable distribution ($M_w/M_n = 2$).

The polymerization actually occurs in three main stages

1. **0 to 0.1% Conversion.** Polymerization occurs only in monomer phase. Because the quantity of polymer produced is so small, this stage can be ignored.
2. **0.1 to 70% Conversion.** Polymerization occurs in both monomer rich and polymer gel phase, but more rapidly in the gel phase.
3. **> 70% Conversion.** Free monomer is exhausted and polymerization occurs in the polymer gel phase of rapidly increasing viscosity as the VCM is consumed. Thus after a further increase in polymerization the rate decreases as the monomer is used up.

1.1.4 Characteristic Properties of PVC

In pure form, PVC is a hard thermoplastic material with a T_g of about 80 °C. It is basically an amorphous polymer. The crystalline melting point is high (about 225 °C). Intrinsically, PVC is a thermally unstable polymer and gives off hydrochloric acid when heated. As dehydrochlorination starts at temperatures much lower than normal processing temperatures, PVC processing requires the use of efficient stabilizers.

1.1.5 Quality Aspects

As with other thermoplastic materials, the molecular weight and molecular weight distribution (MWD) are important quality properties. With PVC, the molecular weight and MWD are determined almost exclusively by chain transfer to monomer, that is, by the polymerization temperature. Some quality properties (i.e., electrical properties, color and thermal stability of the polymer) may be affected by the particular choice of

processing aids and by the exact way in which the process is conducted. The suspension stabilizer system affects the shape of the grains, the grain size distribution, resin porosity and bulk density of resin.

1.1.6 Main Outlets of PVC

PVC is processed either in unplasticized (hard PVC) or plasticized form (flexible PVC). Hard PVC is a hard and tough material. The main outlets for hard PVC are pipes and fittings, extruded profiles, films, bottles, and gramophone records. Flexible PVC is mainly used as film, cable insulation, flooring, leather substitutes, flexible tubing, and extruded profiles.

1.2 Control of PVC reactors

Recent advances in computer technology have made the implementation of modern control algorithms a possibility in industrial environments. Traditionally, chemical processes have been regulated quite successfully with on-off and PID controllers. Many of the modern algorithms, when applied to complex non-linear processes with unmeasurable disturbances have often failed to provide stable and robust control. Nowadays, more effort is being invested in the design of control techniques with improved robustness properties, and some successful applications have already been reported. Several of these applications have shown that adaptive controllers, designed to automatically adjust the controller settings to satisfy a continuously changing environment, can provide a flexible tool to deal with uncertainties, non-linearities and time-varying parameters in a process.

Polymerization of PVC is usually carried out in a batch reactor. The reaction is highly exothermic and is characterised by an auto-accelerating rate profile followed by a

sudden drop in reaction rate at critical conversion. Batch operation and the nature of the rate profile make the process non-linear and time-varying. This makes temperature control of the reactor a challenging control problem.

In the temperature control of exothermic batch reactions, the non-stationarity and non-linearity is linked with the change in rate of heat generation (and therefore the rate of reaction) with time. This is especially so if the heat transfer coefficients and the thermal capacity of the reaction mass do not change drastically during the course of the reaction. If the heat of reaction can be measured, it can be considered as a disturbance and can be explicitly taken care of in the control algorithm.

In this work, the mathematical model used by Kiparissides and Shah (1983), is used. This model was proposed by Abdel-Alim and Hamielec (1972). Eventhough more realistic models have appeared subsequently in literature, this model is used because it captures the essential (from the control point of view) features of the kinetics while retaining a simplicity that makes it easy to simulate; moreover the use of this model enables the comparison of the results with work done previously. We use the Model Predictive Controller (MPC) proposed by Garcia and Morari in both fixed as well as adaptive form to control the PVC batch reactor. The performance of the MPC is evaluated and compared against that of Generalized Predictive Controller, and other adaptive control techniques.

1.3 Proposed Objectives

This thesis has been taken up with the following objectives:

- To develop the mathematical model of the system under study by identification of the process.
- To apply MPC to control the simulated PVC batch reactor under isothermal conditions.
- To apply MPC to control the molecular weight of the PVC subjected to constraints.
- Modify MPC and make it adaptive, by identifying the model parameters on-line after each sampling interval.
- Compare the performance of MPC with other control algorithms that have been studied in literature on control of batch reactor.

1.4 Outline of thesis

In Chapter 2 a detailed survey of literature on PVC modeling and PVC batch reactor control has been given. Chapter 3 contains a short derivation of the MPC algorithm in its linear and nonlinear form, the adaptation algorithm for adaptive MPC and the objectives of MPC. In Chapter 4 we present the mathematical equations of mass and energy balance which model the system under consideration. Chapter 5 discusses the formulation of the control problem and different control strategies adopted, here we also discuss some guidelines for selection of MPC design parameters and methodology of the design decisions. Chapter 6 contains results and discussions of the simulations. In Chapter 7 we have the conclusions that can be drawn from this work and some suggestions for further study.

Chapter 2

Literature Survey

2.1 PVC Modeling

There has been considerable amount of work on the modeling of PVC formation reported in the literature, particularly in developing kinetic mechanisms. These models are all based on the key feature that PVC is essentially insoluble in its monomer so that as polymerization proceeds within the monomer droplets, solid polymer precipitates out and swells to the extent of approximately 23% by weight of VCM to form a deformable viscoelastic gel.

A two phase model (monomer rich phase and polymer rich phase) was first proposed by (Talamini and Pegion, 1966) and this was the first model to predict the rate of polymerization up to 70% conversion. The onset of the two separate phases was reported to begin after less than 1% conversion and lasts until between 70-80% conversion. This particular conversion at which the monomer phase gets depleted is called the critical conversion, x_c . As long as the monomer exists as a separate phase it will exert its vapor pressure and the reactor pressure remains constant during isothermal polymerization; and once conversion exceeds the critical conversion, monomer as a separate phase has been consumed, and the pressure in the reactor begins to fall. The assumptions made in Talamini's model are

1. The corresponding initiator decomposition and propagation rate constants as well as the initiator efficiencies in the two phases are equal.
2. The initiator concentration is the same in both the phases.
3. No transfer of radicals between the two phases occurs.
4. The initiator concentration does not change with conversion.
5. The volume of the reaction mixture remains constant.

Talamini's model was later modified by (Abdel-Alim and Hamielec, 1972) to give conversion more than x_c . This model could also predict the molecular weight distribution (MWD), accurately throughout the entire range of conversions. This model is similar to Talamini with assumptions (4) and (5) replaced by the following two assumptions:

4. The initiator concentration changes with reaction time.
5. The volume of the reaction mixture varies linearly with conversion.

This model assumes the presence of two phases in equilibrium, each of constant composition (x_1 & x_2 % of polymer respectively). x_1 is very small and has been taken as zero, that is, the monomer rich phase contains only monomer.

This two phase model has been further modified by (Ugelstad, 1981) and (Olaj, 1977), but have tended to concentrate on the low conversion behavior. Their models were unable to reproduce a sharply peaked rate feature in the vicinity of so called "pressure-drop region".

A multi-phase mass transfer model (monomer, polymer, VCM droplet surface, aqueous, and vapor phases) has been proposed by (Kelsall and Maitland, 1983). This

model incorporates (a) mass transfer for various species within the different phases involved, and (b) inhomogeneous initiator distribution between monomer and polymer phase and (c) initiator efficiency ratio between monomer and polymer phase. The model can predict rate profile, product MWD and several important properties of product like porosity, apparent density and particle size etc. from a knowledge of process conditions. A number of assumptions which do not necessarily hold for the reacting system, were relaxed by Kelsall & Maitland, like

1. Newly formed polymer is instantaneously swollen to equilibrium conditions by monomer.
2. The initiator is uniformly distributed between the monomer and polymer gel phases.
3. The efficiency of the initiator radicals in initiating polymer chains is the same in both phases.
4. The mass transfer rate between the phases is infinite for monomer, initiator and polymer, but zero for growing radicals.

(Xie et al., 1987) proposed an equilibrium model relating temperature, pressure, monomer conversion, and monomer phase distribution for vinyl chloride polymerization. This model can be used to determine the monomer conversion beyond the pressure drop by measurement of reactor temperature and pressure.

The most recent study on modeling of PVC suspension process was done by (Sidiropoulou and Kiparissides, 1990) where they proposed a new model and compared it with previous four models, of (Abdel-Alim and Hamielec, 1972), (Ugelstad, 1973), (Kuchanov and Bort, 1973) and (Kelsall and Maitland, 1983). They have shown that no

significant difference exists between all these model predictions. But their proposed model can give some new results like, the number of short and long chain branches as well as the number of unsaturated terminal double bonds per polymer molecule.

2.2 PVC Reactor Control

As mentioned earlier the polymerization of PVC is exothermic in nature. During the reaction time reaction temperature must be precisely stabilized by heat removal through the jacket in order to achieve the desired product quality. This constitutes a difficult control problem, mainly due to factors like changing heat transfer coefficient, which varies as much as 30%, change of cooling water temperature, rapid heat generation due to Tromsdorff effect. This makes conventional controller rather unsatisfactory and suggests a self tuning approach. A simulation study by (Kiparissides and Shah, 1983) based on a phenomenological model of the process entirely confirmed the suitability of this approach. They evaluated the performance of two adaptive controllers, the self tuning regulator by (Astrom and Wittenmark, 1973) and globally stable adaptive controller of (Martin-Sanchez, 1976). The two adaptive strategies gave good control of the reactor's temperature and gave better performance than conventional PID controller. (Takamatsu et al., 1986) proposed two kinds of Model Reference Adaptive Schemes for the control of suspension batch polymerization reactor to maintain specific average degree of polymerization and reactor temperature. All predictive control strategies including Generalised Predictive Control(GPC), Model Predictive Control(MPC), Dynamic Matrix Control(DMC), and Model Algorithm Control(MAC) can provide good robust control.

There exists considerable literature on the control of polymerization reactors. Hoogendoorn (1980) surveys the control of commercial continuous and batch polymerization plants, by conventional means as well as by the use of process computers. Another good survey on process computer applications in the polymerization industry has been presented by Amrehm (1977). Keyes and Kennedy (1974) describe an adaptive control technique for control of suspension PVC processes. Gran and co-workers (1974) have used a digital computer to produce a good quality PVC in a production cycle of minimum time duration. Ham and Liemburg (1975) compare five control systems for temperature control of an exothermic simulated batch reactor by applying a quantitative performance criterion.

Kiparissides and Shah (1983) have compared a PID controller with two adaptive controllers for the control of a simulated PVC reactor. Niederlinski (1985) used a cascade PID controller and an adaptive minimum variance controller to control a PVC pilot plant reactor, and found the performance of the adaptive algorithms to be superior to that of the PID controller.

Chapter 3

Model Predictive Control

3.1 Introduction

Model predictive control was conceived in the 1970s primarily by industry. Its popularity steadily increased throughout the 1980s. At present, there is little doubt that it is the most widely used multivariable control algorithm in the chemical process industries and in other areas. This is supported by many reported industrial applications and academic studies (McAvoy et al. 1989). The general strategy of MPC algorithms is to utilize a model to predict the output into the future and minimize the difference between this predicted output and the desired one by computing the appropriate control action. Most of the MPC techniques are used on linear models and are thus not very well suited for the control of nonlinear systems. Because of this, there have been numerous efforts to extend MPC techniques for the control of nonlinear systems. These include the papers by Brengel and Seider (1989), Eaton et. al. (1988), Li and Biegler (1989) and Li et. al. (1990).

While MPC is suitable for almost any kind of problem, it displays its main strength when applied to problems with

- a large number of manipulated and controlled variables;
- constraints imposed on both the manipulated and controlled variables;
- changing control objectives and/or equipment (sensor/actuator) failure;

- time delays.

Some of the popular names associated with model predictive control are Dynamic Matrix Control (DMC), IDCOM, model algorithmic control, etc. While these algorithms differ in certain details, the main ideas behind them are very similar. Indeed, in its basic unconstrained form MPC is closely related to linear quadratic optimal control. In the constrained case, however, MPC leads to an optimization problem which is solved on-line in real time at each sampling interval. MPC takes full advantage of the power available in today's control computer hardware.

3.2 Linear MPC

A brief explanation of this algorithm (for more details see Garcia and Morshedi, 1986) is provided here. The major elements of MPC are

1. The model,
2. Estimation of the disturbance and projection into the future, and
3. Computation of the control inputs.

3.2.1 Modeling

Consider the single-input/single-output (SISO) case, without any loss of generality, The model used is a discrete “**step-response model**” of the form

$$y(k) = \sum_{i=1}^N a_i \Delta u(k-i) + a_N u(k-N-1) + d(k) \quad (3.1)$$

where

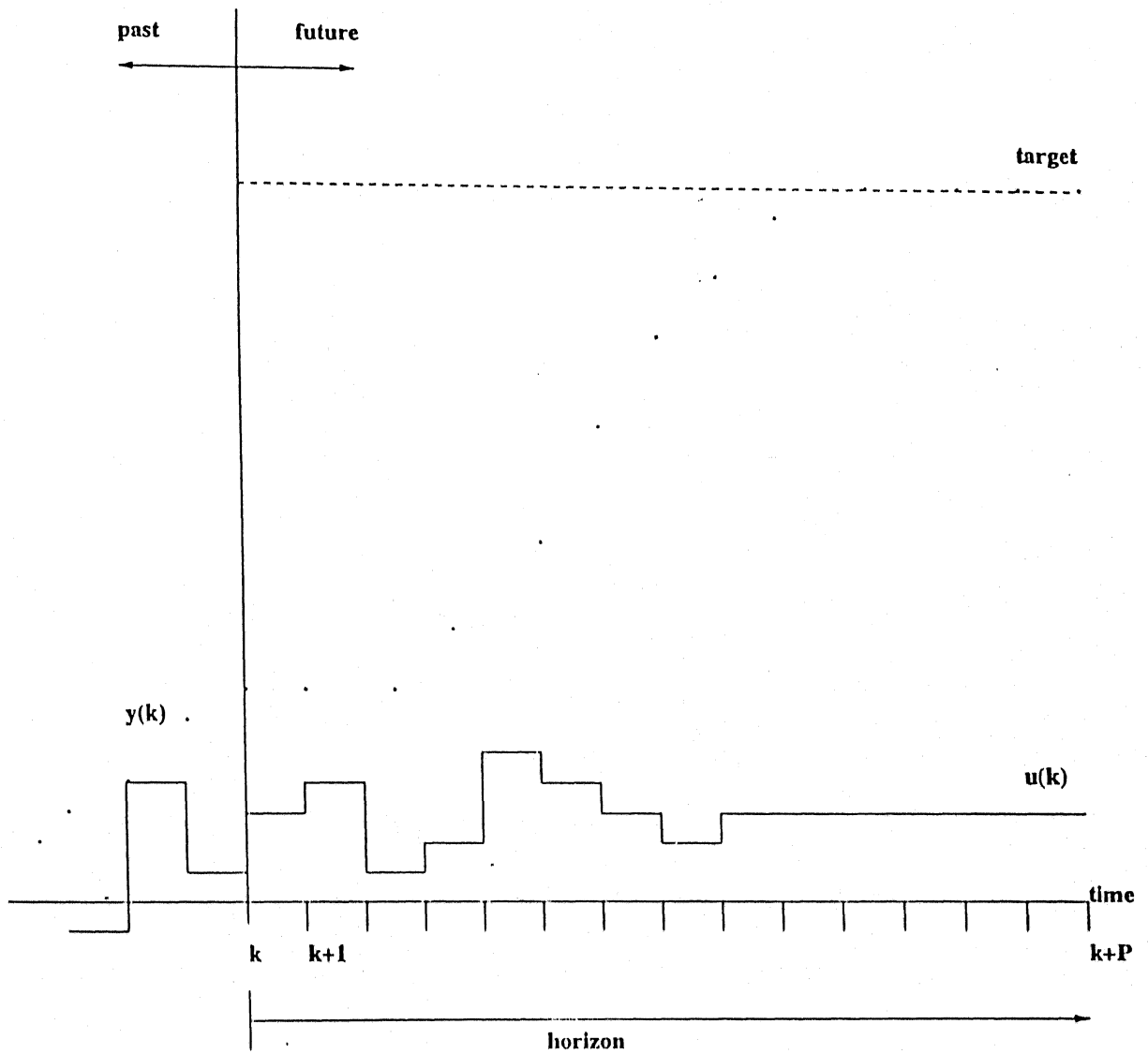


Fig. 3.1: The moving horizon of MPC.

- k is the sampling time
- u is the input
- a_i are the step-response coefficients
- d is the unmodeled or disturbance effects on the output
- N is the number of step-response coefficients needed to adequately describe the process dynamics.
- $\Delta u(k)$ is the change in the input defined as $u(k) - u(k-1)$.

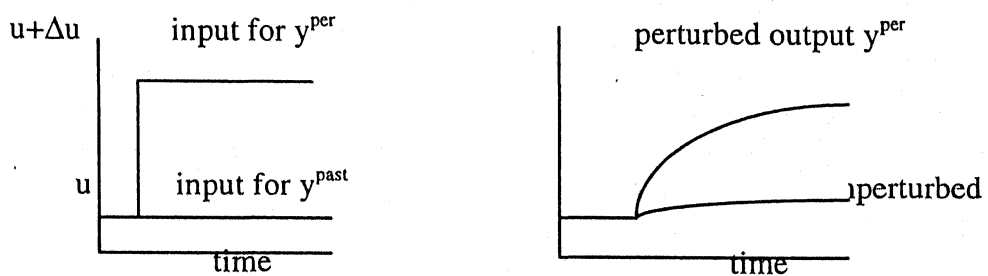


Fig. 3.2: Estimating step- response coefficients.

The step - response coefficients are determined as shown in the Fig. 3.2. Keeping a constant input and integrating forward gives the unperturbed output y^{past} . Stepping the input to a new value and integrating into the future gives the perturbed output, y^{per} . The step - response coefficients are then calculated from

$$a_i = \frac{[y^{per}(k+i) - y^{past}(k+i)]}{\Delta u}$$

3.2.2 Estimation of the disturbance effects

The current value of the disturbance effects can be estimated by subtracting the effects of past inputs on output, from the current measurement of the output, i.e.

$$d(k) = y^{meas}(k) - \sum_{i=1}^N a_i \Delta u(k-i) - a_N u(k-N-1) \quad (3.2)$$

3.2.3 Prediction into the future

The linear estimates of the future output are given by

$$\begin{bmatrix} y(k+1) \\ y(k+2) \\ y(k+3) \\ \vdots \\ y(k+M) \\ \vdots \\ y(k+P) \end{bmatrix} = \begin{bmatrix} a_{ss} u(k-N) \\ a_{ss} u(k-N+1) \\ a_{ss} u(k-N+2) \\ \vdots \\ a_{ss} u(k-N+M-1) \\ \vdots \\ a_{ss} u(k-N+P-1) \end{bmatrix} + \begin{bmatrix} a_2 & a_3 & \cdots & \cdots & a_N \\ a_3 & a_4 & \cdots & a_N & 0 \\ a_4 & a_5 & \cdots & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots \\ a_{M+1} & \cdots & 0 & 0 & \\ \vdots & & & & \\ a_{P+1} & \cdots & 0 & 0 & \end{bmatrix} \begin{bmatrix} \Delta u(k-1) \\ \Delta u(k-2) \\ \Delta u(k-3) \\ \vdots \\ \Delta u(k-N+1) \end{bmatrix}$$

$$+ \begin{bmatrix} a_1 & \cdots & \cdots & 0 \\ a_2 & a_1 & \cdots & \cdots \\ a_3 & a_2 & a_1 & \cdots \\ \vdots & & & \\ a_M & a_{M+1} & \cdots & a_1 \\ a_P & a_{P-1} & \cdots & a_{P-M+1} \end{bmatrix} \begin{bmatrix} \Delta u(k) \\ \Delta u(k+1) \\ \Delta u(k+2) \\ \vdots \\ \Delta u(k+M-1) \end{bmatrix} + \begin{bmatrix} d(k+1) \\ d(k+2) \\ d(k+3) \\ \vdots \\ d(k+M) \\ \vdots \\ d(k+P) \end{bmatrix} \quad (3.3)$$

or,

$$y^{lin} = y^{past} + A \Delta u + d \quad (3.4)$$

- P is the prediction horizon.
- M is the control horizon or the number of future moves $\Delta u(k)$, ..., $\Delta u(k+M-1)$ calculated by the MPC algorithm discussed below.

- A is the dynamic matrix composed of the step- response coefficients. The effects of the known past inputs on the future outputs is defined by the vector y^{past} .

Often the future behaviour of the disturbance is not known, and it is customary to assume that the future values will be equal to the currently estimated value, i.e

$d(k+i) = d(k)$ for $i = 1, \dots, P$ and $d(k)$ is calculated from eq. (3.2).

With these definitions the future output can now be predicted from eq. (3.4) for any given vector of future control moves Δu .

3.2.4 Calculation of the control inputs

The following optimization problem is used to calculate the control inputs:

$$\min_{\Delta u} \sum_{i=1}^P \gamma^2(i) [y^{sp}(k+i) - y^{lin}(k+i)]^2 + \sum_{j=1}^M \lambda^2(j) [\Delta u(k+M-j)]^2 \quad (3.5)$$

- y^{sp} is the set point.
- γ is the time varying weight on output error.
- λ is the time varying weight on the change in the input.

The solution to the above problem is a least - squares solution in the form of the following linear control law:

$$\Delta u = (A^T \Gamma^T \Gamma A + \Lambda^T \Lambda)^{-1} A^T \Gamma^T \Gamma (y^{sp} - y^{past} - d) \quad (3.6)$$

where

- Γ is the diagonal matrix containing weights $\gamma(I)$.
- Λ is the diagonal matrix containing weights $\lambda(I)$.

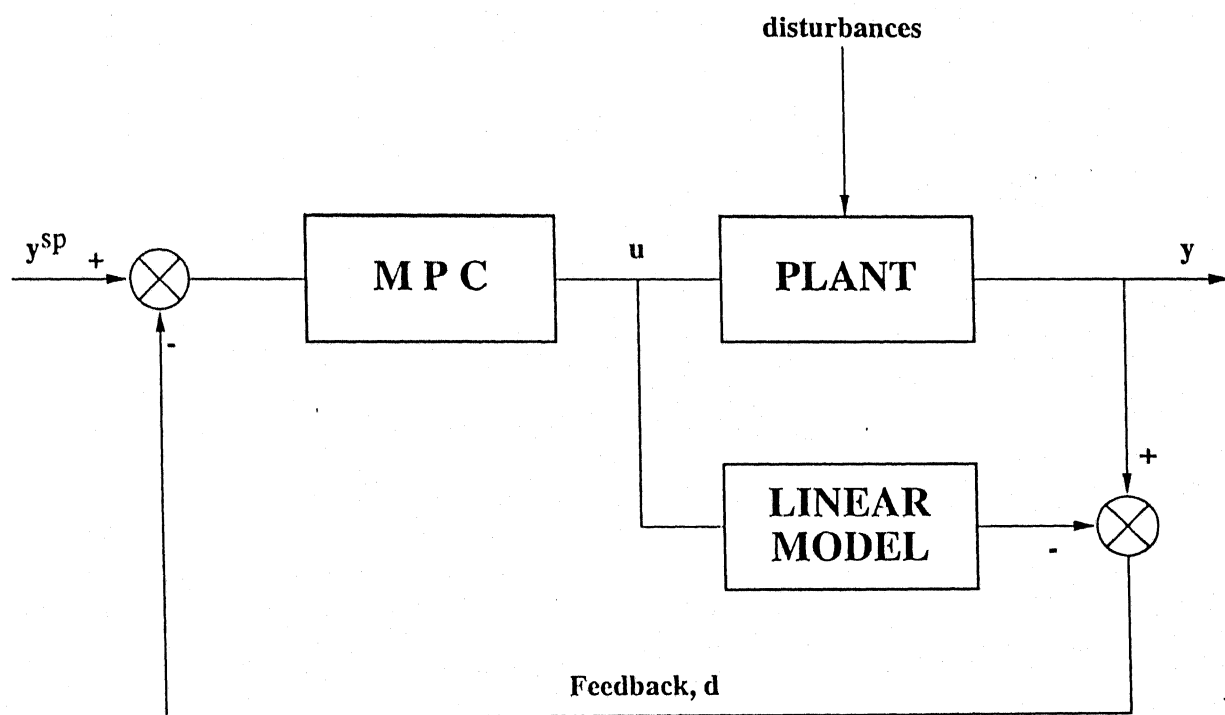


Fig. 3.3: Linear MPC.

Usually only the first calculated move $\Delta u(k)$ is implemented and the calculations are repeated at the next sampling time to account for changing disturbances and to incorporate feedback. P , M , Γ and Λ are used as tuning parameters.

3.3 Nonlinear MPC .

The nonlinear MPC algorithm proposed here stems from reinterpreting the disturbance vector \mathbf{d} appearing in the prediction equations (3.3). If the linear MPC is implemented on a linear plant, the vector \mathbf{d} will contain contributions from nonlinearities defined as \mathbf{d}^{nl} as well as external disturbances defined as \mathbf{d}^{ext} , which is

$$\begin{bmatrix} d(k+1) \\ \vdots \\ d(k+P) \end{bmatrix} = \begin{bmatrix} d^{ext}(k+1) \\ \vdots \\ d^{ext}(k+P) \end{bmatrix} + \begin{bmatrix} d^{nl}(k+1) \\ \vdots \\ d^{nl}(k+P) \end{bmatrix} \quad (3.7)$$

In linear MPC the vector \mathbf{d} and therefore the future disturbance vector due to nonlinearities, \mathbf{d}^{nl} is assumed constant. In the nonlinear MPC formulation, the vector \mathbf{d}^{nl} will be estimated using a nonlinear dynamic model and will no longer be assumed to be constant. The development proceeds as follows:

First, in accordance with eqs (3.4) and (3.7) an extended linear MPC model is defined over the future prediction horizon of length P .

$$y^{el} = y^{past} + A\Delta u + d^{ext} + d^{nl}$$

where \mathbf{d}^{nl} is varying from one sampling time to another, and \mathbf{d}^{ext} is assumed to remain constant over the prediction horizon. The optimal MPC inputs for the extended linear model become

$$\Delta u = (A^T \Gamma^T \Gamma A + \Lambda^T \Lambda)^{-1} A^T \Gamma^T \Gamma (y^{sp} - y^{past} - d^{ext} - d^{nl}) \quad (3.8)$$

The objective is to compute a time - varying disturbance vector, \mathbf{d}^{nl} that captures the future disturbance due to nonlinearities and renders the above $\Delta \mathbf{u}$ optimal for the *nonlinear* model. This is accompanied by requiring the output of the extended linear model (\mathbf{y}^{el}) match the output from the nonlinear model (\mathbf{y}^{nl}) at all the future sampling times:

$$\begin{bmatrix} y^{nl}(k+1) \\ \vdots \\ y^{nl}(k+P) \end{bmatrix} = \begin{bmatrix} y^{el}(k+1) \\ \vdots \\ y^{el}(k+P) \end{bmatrix} = y^{past} + A\Delta u + d^{ext} + \begin{bmatrix} d^{nl}(k+1) \\ \vdots \\ d^{nl}(k+P) \end{bmatrix} \quad (3.9)$$

This is a set of P simultaneous nonlinear equations in P unknowns, $d^{nl}(k+1), \dots, d^{nl}(k+P)$. The quantities \mathbf{y}^{past} and \mathbf{d}^{ext} can be separately calculated as before, and $\Delta \mathbf{u}$ is obtained from eq. (3.8). The terms containing nonlinearities with respect to \mathbf{d}^{nl} appear in the \mathbf{y}^{nl} vector. This is because the output from the nonlinear model will have nonlinear dependence on the input, which in turn depends on \mathbf{d}^{nl} through eq. (3.8).

Any standard nonlinear equation solution method can be used to obtain the vector \mathbf{d}^{nl} satisfying eq. (3.9). One method of doing this is successive substitution or a fixed - point algorithm:

$$d_{l+1}^{nl} = d_l^{nl} + \beta(y_l^{nl} - y_l^{el}) \quad (3.10)$$

where

- l is the iteration number.
- β is a relaxation factor in $(0,1)$ used to enlarge the region of convergence.

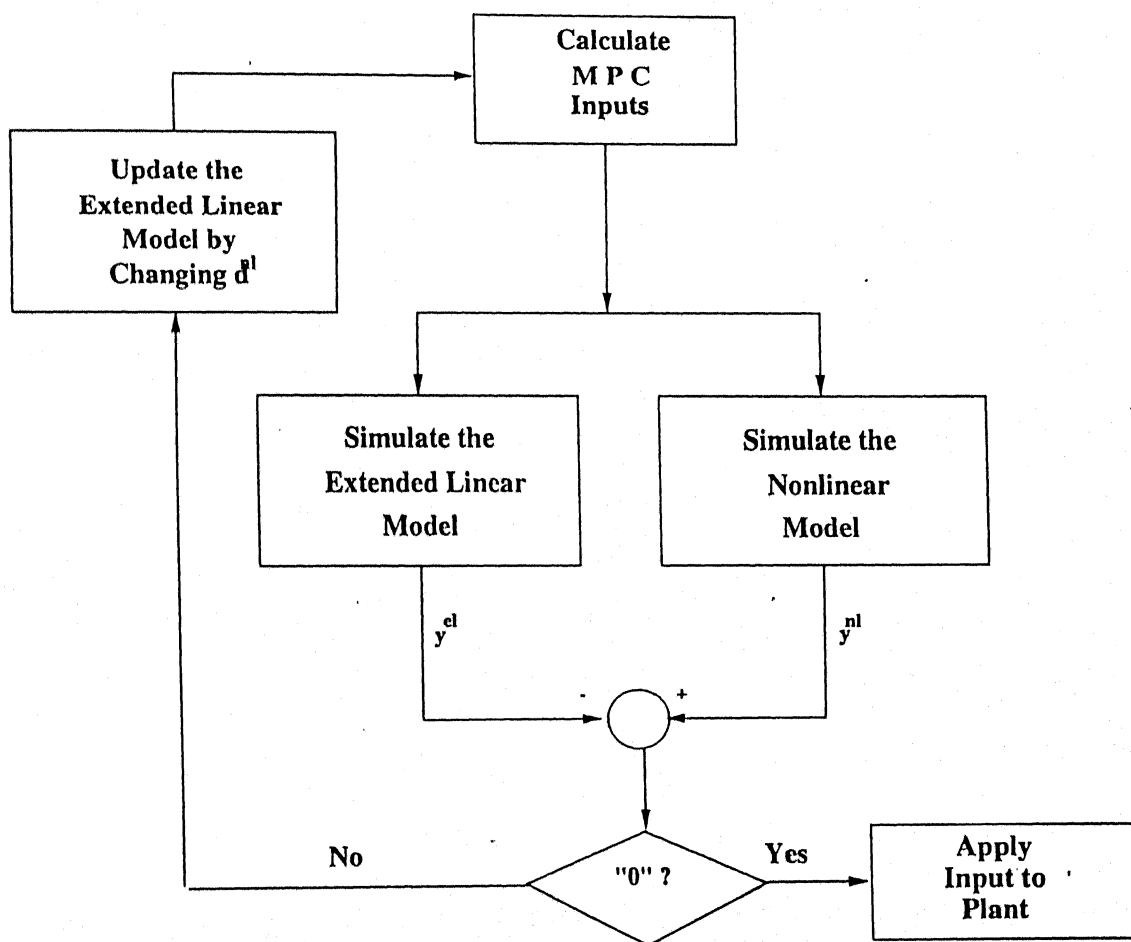


Fig. 3.4: The flow chart of the nonlinear MPC algorithm.

A flow chart for the nonlinear MPC algorithm showing the fixed- point iterations is given in Fig. 3.4. Only the first control action $\Delta u(k)$ is implemented after the iterations (3.10) converge, and the iterative MPC calculations are repeated at the next sampling time.

3.4 Adaptive Algorithm

Adaptive character is given to the prediction controller by an on - line adaptation of the model parameters ie. identification of polynomials $A(q)$ and $B(q)$. MPC uses a model of the plant explicitly to generate the control action. Linear model of the following form is used (for detailed explanation of model see Ch. 5):

$$A(q) y(t) = B(q) u(t - nk) + e(t) \quad (3.11)$$

The model used is linear and can be easily estimated by recursive algorithms. This makes MPC a natural candidate for adaptive control. The recursive algorithms are used to estimate the coefficients of $A(q)$ and $B(q)$.

The recursive least squares (RLS) with exponential forgetting is a commonly used algorithm (Ljung and Soderstrom, 1983) in which older data is given lesser weight. This keeps the algorithm sensitive to any change in parameters and enables identification of non-stationary processes. The tuning parameter of this algorithm is a forgetting factor (denoted by μ). The data j sample instants in the past is given a weight of μ^j , $\mu \leq 1.0$, thus discounting old data exponentially (eqn B.4). It has been observed , (Fortescue, 1981), that in absence of sufficient excitation, the estimator becomes very sensitive to any disturbance or numerical error, and a change in set point or a random input could make the estimator unstable.

In order to avoid these problems the concept of variable forgetting factors has been introduced by (Fortescue, 1981). This is the standard RLS algorithm with exponential forgetting, except that μ is no longer kept constant. It is changed depending on how well the current model fits the new data. If the current model fits the new data well, then $\mu \rightarrow 1$ (slow forgetting), otherwise $\mu < 1$. The tuning parameter in this algorithm is Σ_0 which is the weighted sum of a posteriori error (eqn B.5). The algorithm adjusts μ such that Σ_0 is kept constant.

The variable forgetting factor algorithm keeps the advantage of the fixed forgetting factor algorithm (sensitivity to new data) while avoiding its drawback (instability). Moreover the number of tuning parameters remain the same. A summary of the variable forgetting algorithm is given in Appendix B.

3.5 Control Objectives of MPC

Desirable properties of a MPC controller include many required of any controller. Distinguishing features are the emphasis on satisfaction of constraints, which was one of the major motivations for the introduction of MPC, apart from its implementability. It is interesting to note that, in addition to effective handling of constraints, MPC can stabilize plants which require discontinuous control laws. The following appear to be the most important control objectives:

1. *Stability*: this is, of course, an essential objective.
2. *Performance*: rapidity of convergence to a set point or accuracy in tracking; often measured by a quadratic performance index.

3. *Constraint satisfaction*: controlled system satisfies hard constraints on controlled variables.
4. *Robustness*: maintenance of stability and performance in presence of model error.
5. *Adaptivity*: ability to respond to changing objectives and/or changing plant characteristics.
6. *Implementability*: reasonable on-line computational demands.

Chapter 4

PVC Batch Reactor Model

A brief discussion of the suspension polymerization process and detailed mathematical model of the suspension batch polymerization reactor is described which is being used for the computer simulation.

4.1 Description of the PVC Suspension Process

Polyvinyl chloride is a most unusual and versatile plastic. It can be used in a variety of products - such as waste and water pipes, window frames, decorative moldings and walls, kitchen utensils, and toys. The suspension process is favored because of the relative ease of polymerization control (heat removal and mixing) and the lower cost of separating and drying the resin.

The PVC polymerization is strongly exothermic with a heat of polymerization about $1.74 \times 10^6 \text{ J kg}^{-1}$. Heat removal and control of these reactors is an important research subject. The decrease in heat transfer coefficient is caused by an increase in viscosity and some scale build up. Large heat transfer areas as well as the addition of cooling coils in the reactors and recirculation of the reaction media through external heat exchangers all in combination with a maximum allowable $(T - T_c)$ can increase the removal of reaction heat.

4.2 Mathematical Model of the System

The mathematical model proposed by [Abdel-Alim and Hamielec, 1972] has been used to describe the process during its whole duration as given in [Kiparissides and Shah, 1983]. According to this model monomer conversion in the batch reactor can be expressed as

$$\frac{dx}{dt} = K_1 (1 + Qx)(1 - Bx)^{-\frac{1}{2}} [I_0]^{\frac{1}{2}} \exp(-k_d t / 2) \quad (4.1)$$

where

$$K_1 = k_p (2fk_d / k_t)^{\frac{1}{2}} \quad (4.2)$$

$$Q = [P(1 - x_c) - 1] / x_c \quad (4.3)$$

the remaining terms are defined in Table 4.1. The kinetic parameters P and x_c can be expressed as a function of temperature

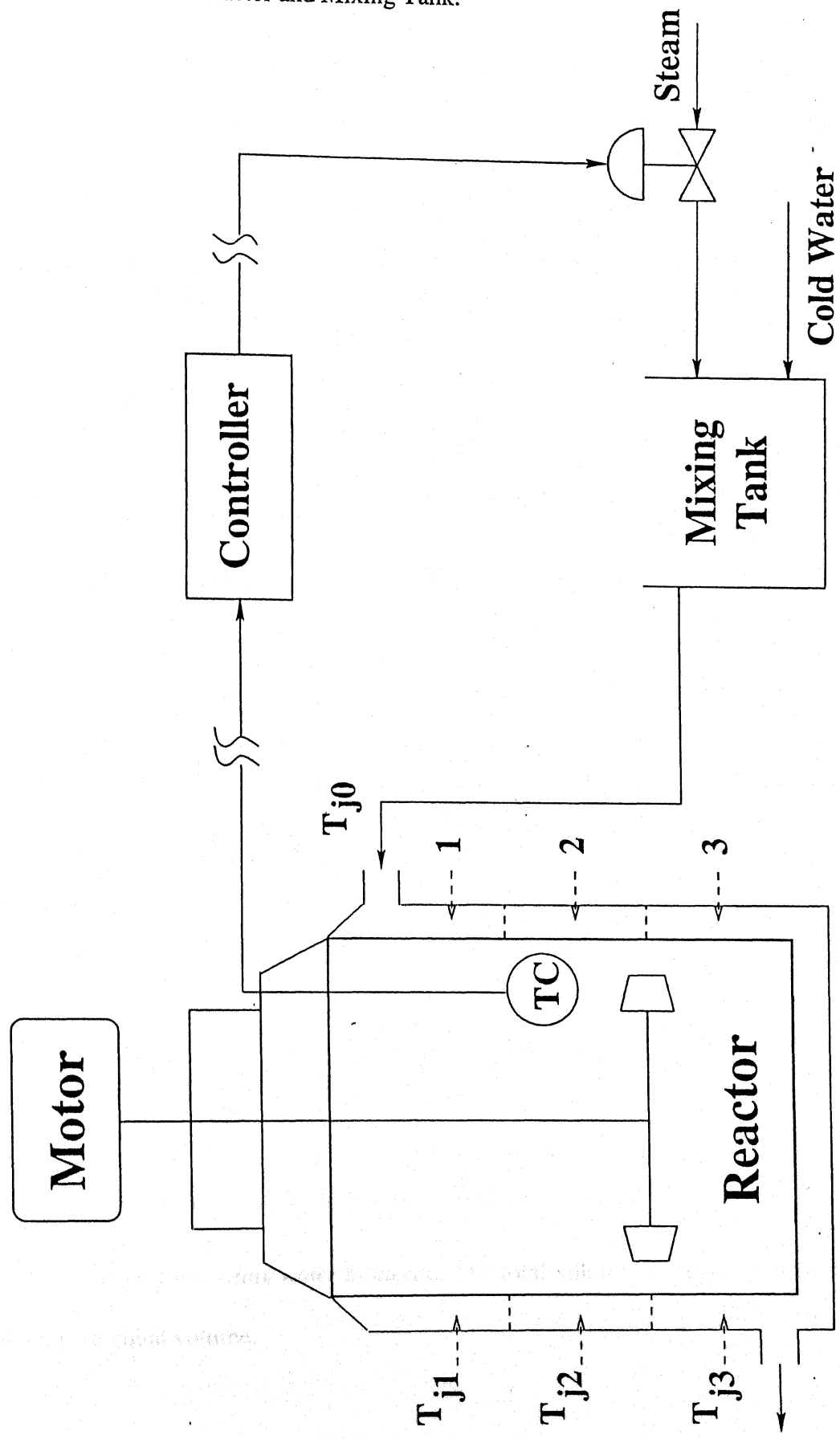
$$P = 27.0 - 0.14(T - 273.16) \quad (4.4)$$

$$x_c = 0.85 - 1.9 \times 10^{-3}(T - 273.16) \quad (4.5)$$

where T is the absolute reaction temperature. Equation (4.1) describes the polymerization in the conversion interval $0 \leq x \leq x_c$. At higher conversion $x_c < x \leq 1$ the following equation represents the kinetics of the polymerization.

$$\frac{dx}{dt} = K_1 P(1 - x)^2 (1 - x_c)^{-1} (1 - Bx)^{-\frac{1}{2}} [I_0]^{\frac{1}{2}} \exp(-k_d t / 2) \quad (4.6)$$

Fig. 4.1: Schematic of Reactor and Mixing Tank.



It has been shown (Abdel- Alim and Hamielec, 1972, 1974) that (4.1) - (4.6) can accurately describe the polymerization kinetics of vinyl chloride for both bulk and suspension processes.

Figure 4.1 presents a simplified diagram of the reactor system under study. Reactants (water, vinyl chloride and initiator) are loaded in the reactor and temperature is raised to the desired value (heating phase). In order to remove the polymerization heat, water is circulated through the jacket of the reactor (stationary phase). The temperature of the cooling water stream is controlled by manipulating the steam flow rate into the premixing tank while keeping the flow rate of the second stream (cold water) constant.

For the nonisothermal polymerization of vinyl chloride in a batch reactor, an overall energy balance around the reactor - cooling system yields the following dynamic equations.

Reactor liquid energy balance : Perfect mixing, constant holdup and constant physical properties are assumed in the reactor.

$$V\rho_m C_p \frac{dT}{dt} = (-\Delta H)[M_0]V \frac{dx}{dt} - h_i A_i (T - T_M) \quad (4.7)$$

Reactor metal wall energy balance : The metal of the reactor wall is treated as a lumped system

$$\rho_M C_M V_M \frac{dT_M}{dt} = h_i A_i (T - T_M) - h_o A_o \times [T_M - \frac{1}{3}(T_{J1} + T_{J2} + T_{J3})] \quad (4.8)$$

Energy equations for cooling water in jacket : The total volume of jacket is divided into three parts of equal volume.

$$\frac{1}{3} V_j r_w C_w \frac{dT_{J1}}{dt} = m C_w (T_{J0} - T_{J1}) + \frac{1}{3} h_0 A_0 (T_M - T_{J1}) \quad (4.9)$$

$$\frac{1}{3} V_j r_w C_w \frac{dT_{J2}}{dt} = m C_w (T_{J1} - T_{J2}) + \frac{1}{3} h_0 A_0 (T_M - T_{J2}) \quad (4.10)$$

$$\frac{1}{3} V_j r_w C_w \frac{dT_{J3}}{dt} = m C_w (T_{J2} - T_{J3}) + \frac{1}{3} h_0 A_0 (T_M - T_{J3}) \quad (4.11)$$

Energy equation for stream mixing tank :

$$\frac{dT_{J0}}{dt} = \frac{1}{d_1} (T'_{J0} - T_{J0}) \quad (4.12)$$

where

$$(T'_{J0} - T_0)(\dot{m}_w + \dot{m}_s)C_w = \dot{m}_s(\Delta H_s) \quad (4.13)$$

Thermocouple system dynamics : A time lag in temperature measurement is described by

$$\frac{dT_h}{dt} = \frac{1}{d_2} (T - T_h) \quad (4.14)$$

T_h is the temperature equivalent of the thermocouple output. The meaning of the symbols in (4.1) - (4.14) and their numerical values as used in the simulation studies are given in Table 4.1. Equations (4.1) - (4.14) constitute the mathematical model of the reactor. Solved simultaneously, they give us the temperature distribution over the reactor - cooling system and the monomer conversion in the reactor. These equations are used to simulate the dynamics of the suspension PVC process.

4.3 Modeling of Molecular Weight

The kinetic model for Suspension Polymerization of Vinyl Chloride given by (Abdel - Alim and Hmielec, 1972) has been used to get the weight and number average

molecular weight equations. It assumes the presence of two phases in equilibrium, each of constant composition (x_i and x_r % of polymer respectively). x_i is very negligible, so it is taken as zero, i.e. the monomer rich phase contains only monomer.

Only relevant equations are being given here (for detailed modeling see Abdel - Alim and Hamielec, 1972).

$$\tau_1 = C_M + \frac{fk_d I_0^{1/2}}{k_1 \sqrt{1-Bx}} \cdot \exp(-k_d t / 2) \quad (4.15)$$

$$\tau_2 = C_M + \frac{fk_d \rho_m I_0^{1/2}}{Pk_1 \rho_2 (1-x_c) \sqrt{1-Bx}} \cdot \exp(-k_d t / 2) \quad (4.16)$$

and for $0 \leq x \leq x_c$,

$$m_1 = \frac{(Qx_c + 1) \ln(1 + Qx) - Qx}{Q^2 x x_c} \quad (4.17)$$

$$m_2 = \frac{P(1-x_c)[Qx - \ln(1 + Qx)]}{Q^2 x x_c} \quad (4.18)$$

while after critical conversion x_c

$$m_1 = (m_1)_{x=x_c} \cdot \frac{x_c}{x} \quad (4.19)$$

$$m_2 = \frac{P(1-x_c)[Qx_c - \ln(1 + Qx_c)] + Q^2 x_c (x - x_c)}{Q^2 x x_c} \quad (4.20)$$

where m_1 and m_2 are the mass fraction of the polymer produced in monomer rich and polymer rich phases.

The number average and weight average molecular weight distributions given by (Xie and Hamielec, 1991) are as

$$\frac{d\bar{M}_w}{dt} = \frac{dx/dt}{x} * (M_w - \bar{M}_w) \quad (4.21)$$

$$\frac{d\bar{M}_n}{dt} = \frac{dx/dt}{x} * \bar{M}_n * (1 - \bar{M}_n / M_n) \quad (4.22)$$

where M_w and M_n are instantaneous molecular weights of polymer given by

$$M_n = \frac{62.5}{m_1\tau_1 + m_2\tau_2} \quad (4.21)$$

$$M_w = 62.5(2m_1/\tau_1 + 2m_2/\tau_2) \quad (4.22)$$

eqns. (4.21) and (4.22) are used for the molecular weight distribution throughout the course of reaction in the simulation runs.

Table 4.1: Physical and design parameters

| Parameter values for the reaction | |
|-----------------------------------|--|
| B | constant in eqn (4.1), $B = (d_p - d_m)/d_p$ |
| d_m | density of monomer, $[947.9 - 1.89(T - 273.16)] \text{ kg/m}^3$ |
| d_p | density of polymer, 1400.0 kg/m^3 |
| $[I_0]$ | initial initiator concentration, 0.03 kmol/m^3 |
| k_d | initiator decomposition rate constant, $1.825 \times 10^{-6} \exp[-15460.5(1/T - 1/323.16)] \text{ s}^{-1}$ |
| K_1 | rate constant defined in eqn (4.2) $9.794 \times 10^{-5} \exp[-8594.8(1/T - 1/323.16)] (\text{dm}^3/\text{mol})^{0.5} \text{ s}^{-1}$ |
| k_p | rate constant of polymer propagation, $\text{dm}^3/\text{mol s}$ |
| k_t | rate constant of polymer termination, $\text{dm}^3/\text{mol s}$ |
| $[M_0]$ | initial monomer concentration, 5.05 kmol/m^3 |
| x | monomer conversion, dimensionless |
| x_c | critical monomer conversion, dimensionless |
| $(-\Delta H)$ | heat of reaction, 106.0 kJ/mol |
| Design parameters | |
| A_i | ($\approx A_0$) inside heat transfer area of the wall, 7.8 m^2 |
| V | reaction volume, 2.0 m^3 |
| V_M | volume of reactor metal wall, 0.1 m^3 |
| V_j | volume of reactor jacket, 0.5 m^3 |
| Physical parameters | |
| C_p | heat capacity of reaction mixture, $3.32 \text{ kJ/kg } ^\circ\text{C}$ |
| C_M | heat capacity of metal wall, $0.48 \text{ kJ/kg } ^\circ\text{C}$ |
| C_w | heat capacity of coolant water, $4.18 \text{ kJ/kg } ^\circ\text{C}$ |
| d_1 | time constant of mixing tank, 20 s |
| d_2 | time constant of thermocouple, 30 s |
| h_i | inside heat transfer coefficient, $1000 \text{ W/m}^2 \text{ } ^\circ\text{C}$ |
| h_o | outside heat transfer coefficient, $2000 \text{ W/m}^2 \text{ } ^\circ\text{C}$ |

continued from previous page

| | |
|----------------|---|
| m | total mass flow rate through jacket, kg/s |
| m_s | variable steam flow rate into mixing tank, kg/s |
| m_w | constant coolant water mass flow rate into mixing tank, 49.75, kg/s |
| T | reaction temperature, °K |
| T_h | thermocouple temperature, °K |
| T_M | metal wall temperature, °K |
| T_c | constant temperature of coolant water entering mixing tank 293 °K |
| T_j | temperature of water in jacket |
| ρ_m | density of reaction mixture, 982.0 kg/m ³ |
| ρ_M | density of reactor wall, 7850.0 kg/m ³ |
| ρ_w | density of coolant water, 995.0 kg/m ³ |
| (ΔH_s) | enthalpy change of steam 2530.0 kJ/kg |

Chapter 5

Control Problem Formulation

This chapter gives a brief outline of the reactor model and the control objectives. The various control strategies adopted and selection of the design parameters are discussed. Selection of tuning parameters in MPC and some tuning guidelines are also presented here.

As mentioned earlier VCM polymerization process is characterized by large amount of heat liberation (106 kJ/mol). Such reactions pose a serious control problem due to the following factors:

1. Non stationary process dynamics caused mainly because of decrease in heat transfer coefficient between bulk and jacket during the polymerization. The heat transfer coefficient may decrease as much as 30-40 %.
2. Rapid change of main disturbance which is the heat generation rate. At conversions around 65-75 % the rate of polymerization is subject to an auto acceleration resulting in a quick increase followed by a quick decrease due to the decrease of monomer concentration.

Process dynamics change from batch to batch due to ageing phenomena (e.g. reactor scaling) or due to different production targets. It is very clear that temperature control is very important to keep the reaction away from runaway conditions. Also it is

clear that temperature is having direct effect on the rate and conversion profile. Other than these, temperature affects all the product properties including molecular weight distribution (MWD), polydispersity index (PDI), porosity, density, and particle size distribution.

5.1 The Model

The schematic diagram of the reactor model has been given in Fig(4.1). The equations describing the kinetics and heat transfer are given in Ch. 4. The reactor is taken to be well mixed, and the heat of reaction is removed by water in the jacket of the reactor. The inlet temperature of the water in the jacket is manipulated by controlling steam flow rate into a premixing tank. The premixing tank has two in-flowing streams, steam and cold water. The flow rate of cold water is kept constant, while steam flow rate is manipulated by controller.

The model by Abdel- Alim and Hamielec (1972) has been used to describe the kinetics of suspension polymerization of PVC in the batch reactor. At critical conversion (approx. 75%), there is a sudden drop in reaction rate due to depletion of monomer. The rate of reaction is given by a single ordinary differential equation in each of the regimes pre x_c and post x_c . In Fig 5.1 the variation of reaction rate is shown when reactor is operated isothermally. The peak in the rate occurs at critical conversion.

The jacket is modeled as if it has 3 distinct zones each of which are well mixed and at an uniform temperature. The jacket side heat transfer coefficient is taken to be constant, so the energy balance for the coolant is described by coupled linear ordinary differential equations.

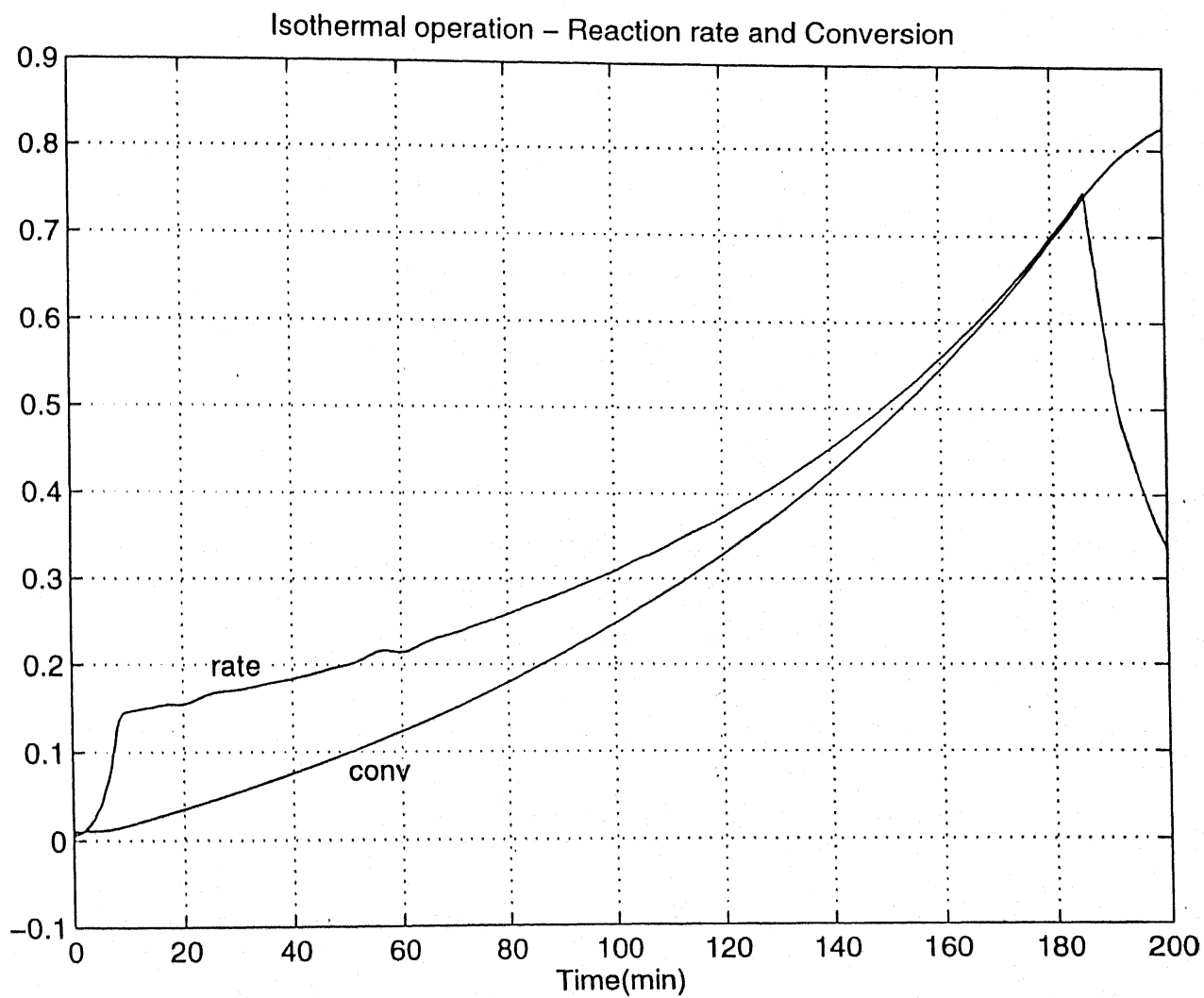


Fig. 5.1: Reaction rate profile when reactor is operated isothermally at 55 °C.

5.2 Control Objectives

In this work we are interested in two problems; first is isothermal control of PVC reactor and second is molecular weight control of PVC. The objectives of the present study are the following:

1. **Develop Process Model:** We develop a mathematical model of the highly nonlinear and time varying process by identification of the process. This model is used in MPC to calculate the control actions.
2. **Constant Temperature Control:** The temperature of the reactor is measured by a thermocouple of known dynamics. Two cases are considered:
 - (a) *Deterministic:* The temperature measurement is accurate and not corrupted by noise.
 - (b) *Stochastic:* The temperature measurement is corrupted by additive white Gaussian noise. Here again we consider two cases:
 - i. The noisy measurement is used 'as is' to calculate the control action.
 - ii. The noisy measurement is passed through a filter in order to attenuate its high frequency components.
3. **Molecular Weight Control:** Here we assume that the molecular weight of polymer can be measured within 5 min (which is sampling time) using any standard technique like, Gel Permeation Chromatography(GPC). The measurement is taken to be exact and uncorrupted by noise. The objective is to put the constraint on molecular weight in order to achieve the PVC of desired molecular weight at the end of the reaction.

5.3 Control Strategies

For both temperature and molecular weight control the manipulated variable is the mass flow rate of steam into the mixing tank. The steam flow rate varies between 0 and 10 kg/s. In this work we apply the MPC in two ways:

Fixed MPC (FMPC): MPC algorithm requires the model of the plant in the form of step - response coefficients to evaluate the control inputs. For this we do the off-line identification of the process using set of input -output data, and get the parameters of the model. These parameters are used to generate the step - response coefficients, which constitutes the model of the process. No modeled disturbances are considered.

Adaptive MPC (AMPC): The plant model is estimated on - line. We do on line identification of the process and step-response coefficients are kept updated at a specified interval of time. This is the adaptive mode of MPC.

5.4 Selection of Tuning Parameters in MPC

Several parameters must be specified to design the MPC controller. It is the proper selection of MPC parameters which ensures the success of MPC in any chemical engineering system. The various tuning parameters are:

1. Sampling time, T_s
2. Process model truncation horizon, NT
3. Output prediction horizon, P
4. Control move horizon, M
5. Weighting on input & output ($\lambda ; \gamma$)

6. Filter

Several authors have suggested guidelines for tuning of these parameters (Cutler, 1983; Marchetti et. al., 1983; Maurath et. al., 1988; Lee and Yu, 1993). For open loop stable plants, nominal stability of the closed - loop system depends only on gain matrix (K_{mpc}), which in turn is affected by the horizon P , the number of moves M , and the weighting matrices γ and λ . No precise conditions on M, P , γ and λ exist which guarantee closed -loop stability.

5.4.1 Selection of T_s and NT

NT is the number of sampling time intervals required for the system to reach steady state. The choice of T_s and NT are interrelated and affect the choice of P . For a self - regulating system the settling time, $T_s * NT$, is finite. The value of NT must be large enough to reduce the truncation error to an acceptable level. Use of small settling time introduces modeling error. Small value of NT is desirable to reduce computation but on the other hand, large T_s reduces controller flexibility and usually results in poor disturbance rejection capability. The product of T_s and NT should be larger than the time required for the open - loop response to reach 95 % of its steady state value. Selection of T_s and NT also decides the number of step - response coefficients to be used in the simulation.

5.4.2 Selection of prediction horizon, P

Increasing the prediction horizon P , has a stabilizing effect on the closed loop system. But increasing P also increases the number equations in the least - squares optimization. The stability of the controller is ensured in MPC when $P \gg M$ (Garcia and Morari, 1982). Garcia and Morshedi (1986) suggested $P = NT + M$.

5.4.3 Selection of control horizon, M

As M is increased, more degrees of freedom are available for controller optimization. This often results in tighter control of the process. Increasing M may result in better control system performance, but at expense of larger changes in the manipulated variable and the controller robustness is reduced. Large value of NT and M make the implementation of MPC impractical because: (a) it requires high computational effort; and (b) it results in poorer controller performance. Cutler (1983), presented a method for selecting M . For selected values of T_s , NT and P with $\lambda = 0$, the value of M is increased until change in M has no further effect on the first move of the controller in response to a step change in set point. This final value of M is taken as the control horizon in the MPC.

5.4.4 Selection of control move suppression factor, (λ)

This parameter is used in the objective function to weight the changes in the input. The selection of λ is usually done experimentally by trial and error using simulation results to judge whether the controller is too sluggish or too fast. Increasing λ reduces the controller gain, slows down the closed-loop response and reduces the size of the input changes and therefore, increases robustness of the controller.

5.4.5 Selection of filter time constant

Noise filter time constant, and the disturbance time constant do not affect closed-loop stability or the response of the system to setpoint changes or measured disturbance. Increasing the noise filter time constant makes the system more robust and the unmeasured disturbance response more sluggish. Increasing the disturbance time constant increases the lead in the loop, making the control action somewhat more aggressive and is recommended for disturbances which have slow effect on the output.

5.5 Design Decisions

Before implementing a controller it is necessary to fix several design parameters : related to the representation model of the process and needed by the identification method and by the controller itself.

5.5.1 Sampling time

- **Temperature Control:** In case of temperature as a controlled variable the sample time was chosen to be 30 seconds. This is the sampling interval chosen in literature for control studies on this system (Ritwik Bhatia, 1996), (Kiparissides and Shah, 1983), (Cluett, 1985). The rise time of this plant is approximately 200 sec, so the sample time falls within the range suggested in (Astrom and Wittenmark, 1990), i.e sample time should be between 1/4 and 1/10 of the rise time of the plant.
- **Molecular Weight Control:** The measurement of molecular weight of any polymer is done off-line in a laboratory, and this analysis requires more time in comparison to the temperature measurement which can be done within few seconds. Keeping this in mind the sampling time for molecular weight control has been chosen 5 min. Gel Permeation Chromatography (GPC) is extensively used with a variety of detectors to obtain molecular weight.

5.5.2 Model structure selection and validation

Once the data have been gathered and the model structure selected, the next step is to select the model parameters that yield the 'best' model. We take the ARX model of the form

$$A(q) y(t) = B(q) u(t - nk) + e(t) \quad (5.1)$$

where B and A are polynomials in the delay operator q^{-1} .

$$A(q) = 1 + a_1q^{-1} + \dots + a_{na}q^{-na} \quad (5.2)$$

$$B(q) = b_1 + b_2q^{-1} + \dots + b_{nb}q^{-nb} \quad (5.3)$$

- na is order of polynomial A .
- nb is order of polynomial B .
- nk is number of delays from input to output.
- $e(t)$ is the white noise.

An ARX model is fitted to the data set, for different structures having different orders and delays. For each of these models, the sum of squared prediction error is computed and the one with smallest Final Prediction Error(FPE) is chosen. A polynomial of third order, B polynomial of second order and dead time of first order has been selected as model orders for both FMPC and AMPC. The order of polynomials used is given in Table 5.1.

| Case | nk | na | nb |
|------|------|------|------|
| AMPC | 1 | 3 | 2 |
| FMPC | 1 | 3 | 2 |

Table 5.1: Order of polynomials $A(q^{-1})$, and $B(q^{-1})$

The values of the coefficients used for FGPC is given in Table 5.2 for different cases under study. In case of temperature control there is one A polynomial of third order, and two B polynomials of second order each corresponding to two inputs steam and cold water respectively. While in case of molecular weight control there is first set of A polynomial corresponding to M_w and B polynomial from steam and second set of A polynomial corresponding to M_n and B polynomial from cold water as an input.

| Case | dead time | a_1, a_2, a_3 | b_1, b_2 |
|----------------------------|-----------|--------------------------|------------------------------------|
| Temperature control | 1 | -2.4500, 1.9472, -0.4972 | 0.0993, -0.0921 -0.0077, 0.0052 |
| Molecular weight (M_w) | 1 | -2.8546, 2.7281, -0.8734 | -1.8813, 0.0607 |
| Molecular weight (M_n) | 1 | -2.8636, 2.7580, -0.8940 | 0.3761, -1.0699 |

Table 5.2: Parameter values of $A(q^{-1})$, $B(q^{-1})$ for FMPC

5.5.3 Set point trajectory

It is the time varying vector of future reference values (set points) used in optimization of the objective function. If one wants the set points to be constant for the entire time, in that case only one value of set point is specified. We use the following equation to generate the set point trajectory for temperature as a controlled variable during the initial heating phase. Here we use one parameter α , in the equation which

decides the nature of trajectory. By changing the value of α the set point trajectory changes.

$$r(k+1) = \alpha * r(k) + (1 - \alpha) * r_{sp} \quad (5.4)$$

where

- r_{sp} is the set point value.
- α is a parameter in the range $0 \leq \alpha \leq 1$.

Chapter 6

Results and Discussion

In this chapter we present the results of the simulation runs performed for different cases under study. All the simulations were done in MATLAB & SIMULINK. The codes are in MATLAB language (M - files) and simulations are performed in SIMULINK using any of the standard integration routines available.

Description of the various terms used for design and tuning parameters presented in the Tables of this chapter is as follows:

- *Step response coefficients*: These represent the model that is to be used for state estimation in the controller.
- *Sampling period (T_s)*: Sample time used.
- *Control horizon (M)*: Number of control moves.
- *Prediction horizon (P)*: Output prediction horizon.
- *Weights on input variables (λ)*: First column is weight on steam(u_1), and second column is weight on cold water(u_2).
- *Constraints on input*: This shows the lower and upper limits on manipulated variable (u_1).
- *Constraints on output*: Lower and upper limits on output variable.

- *Parameter α* : This is used to determine the nature of set point trajectory for controlled variable (Eqn. 5.4).
- *tfilter*: It is a matrix of time constants for the noise filter and the unmeasured disturbances.

6.1 Constant Temperature Control

In this section we discuss the results of the simulations when we try to maintain the reactor temperature at a constant value of 55 °C. First of all the step response model of the system is presented, which has been developed by identification of the input-output data. We consider both controlling schemes, fixed and adaptive (FMPC & AMPC) under various conditions - deterministic, stochastic (without filtering of noise) and stochastic (with filtering). MPC design parameters are also presented here under different cases considered.

6.1.1 Step response model

Step response model of the system is shown in Fig. 6.1 and 6.2. First set is step response of u_1 (steam) and second set is step response of u_2 (cold water). The number of step response coefficients have been selected as 95 after which values becomes constant. During simulation steam flow rate (u_1) is manipulated by the controller while cold water (u_2) is passed at a constant rate of 49.75 kg/sec. Throughout the discussion of results in this chapter input variable means - steam flow rate, which is the manipulated variable of the controller and cold water is kept at a constant value.

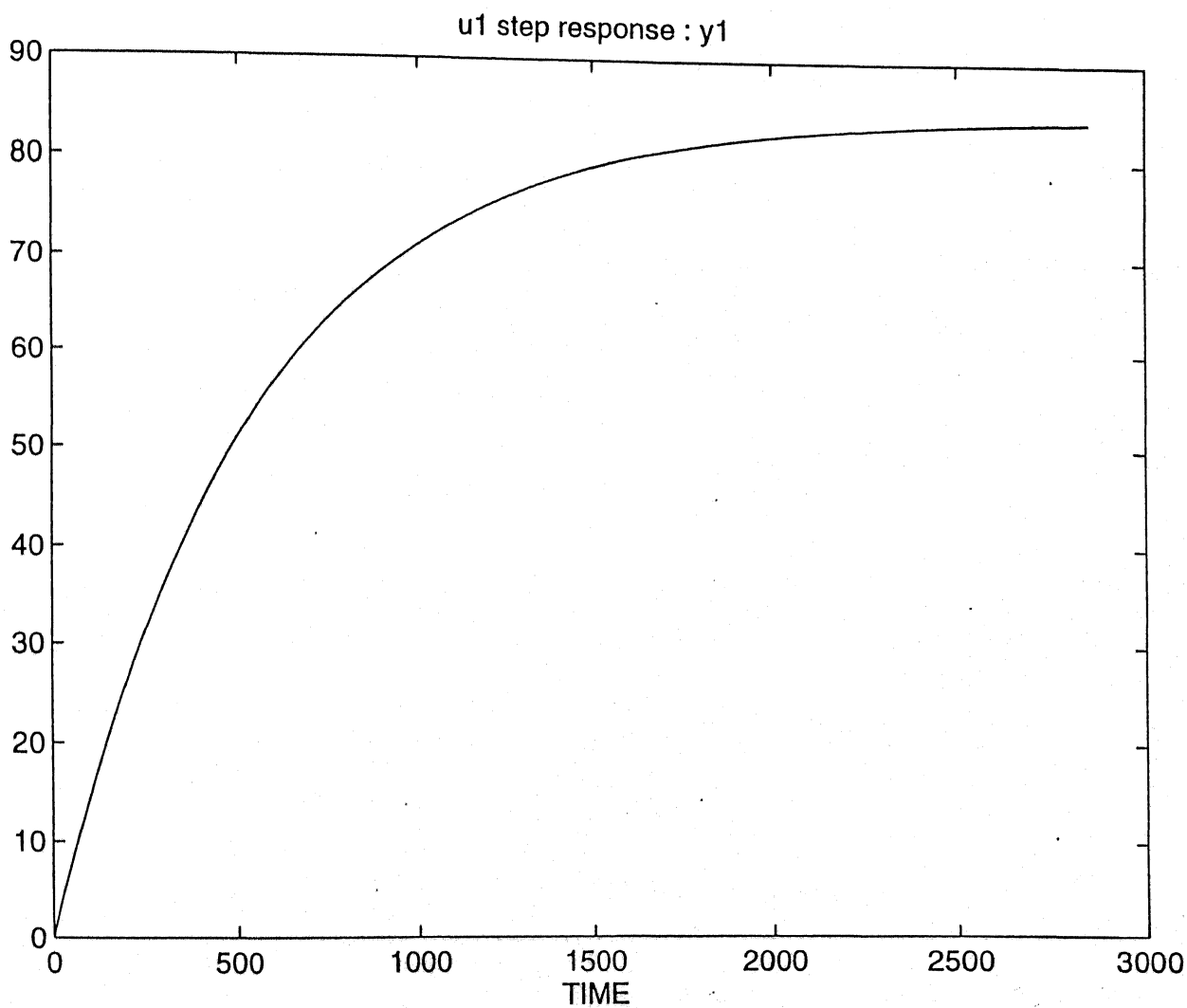


Fig. 6.1: Plot of Step Response

u_1 - steam flow rate, y_1 - reaction temperature

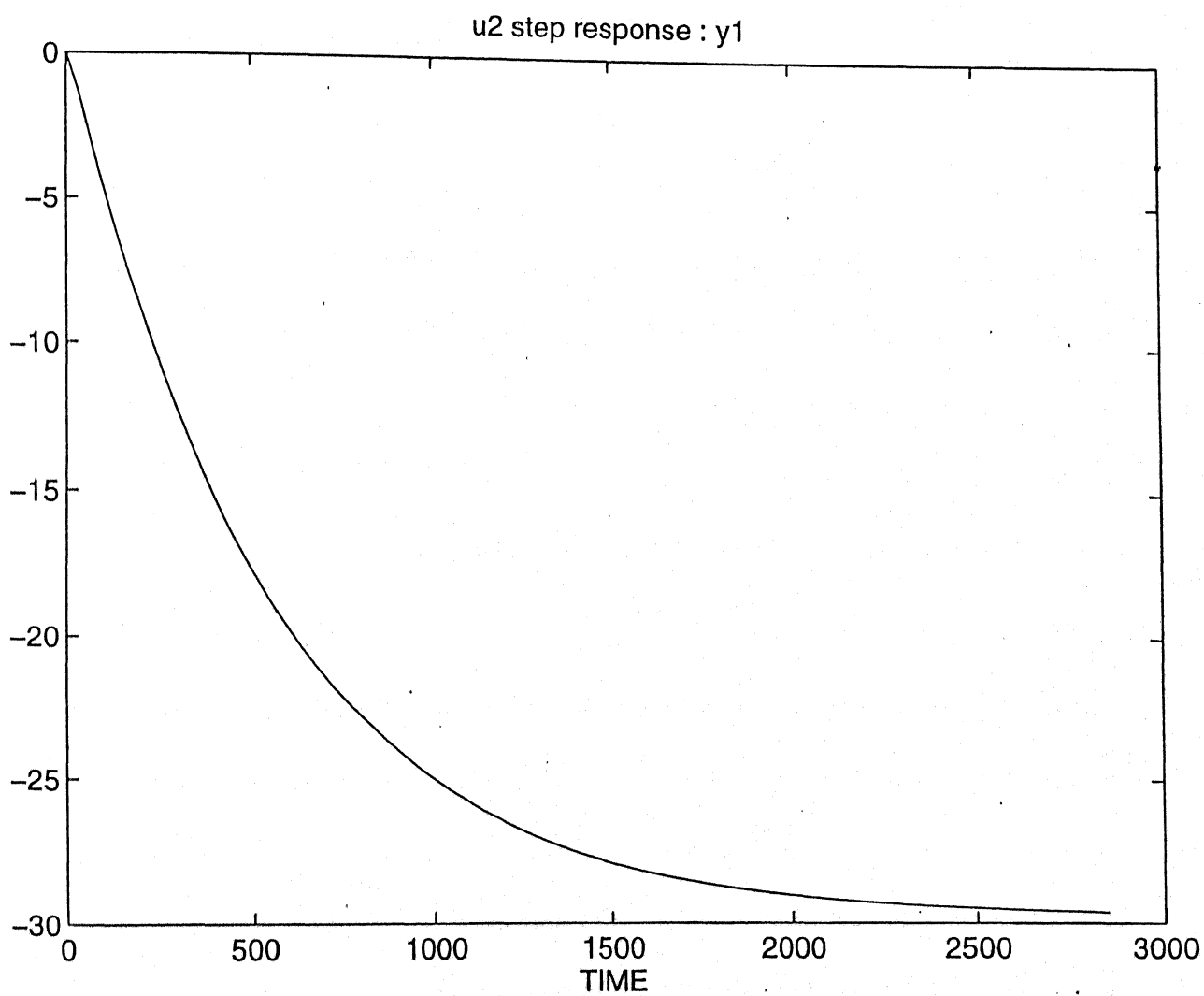


Fig. 6.2: Plot of Step Response

u_2 - cold water flow rate, y_1 - reaction temperature

6.1.2 Deterministic

- FMPC:** In the deterministic case (no noise in temperature measurement), the design parameters of FMPC are given in Table 6.1. In this case control horizon $M=1$, and prediction horizon $P=10$, have been chosen as suitable values. These low values of M and P are the key factor for the quick calculation of the controller action. Constraints on input and output shows the lower and upper limits respectively. The selection of the weights on input variables was the most important factor, finally selected values for this case are listed in the Table 6.1. First value of λ corresponds to u_1 and second value corresponds to u_2 . The values of the coefficients of A and B polynomial are given in the previous chapter in Table 5.2. Fig. 6.3 shows the controlled variable (temperature) and manipulated variable (steam) profile throughout the course of reaction. The time constant of the filter for unmeasured disturbances entering the plant has been taken as 9 sec(second column of t_{filter} in the Table 6.1). The value of parameter α , used in determining the set point trajectory (Eqn. 5.4) has been chosen to be 0.921.
- AMPC:** In adaptive MPC the number of step response coefficients have been chosen as 25, and these are kept updated after every sample time. This was chosen after observing the values of the coefficients, which were found to be constant after 25. Control horizon, $M=1$ and prediction horizon, $P=24$ were found most suitable as shown in the Table 6.2. Time constant of the filter for unmeasured disturbances was chosen as 5 sec. However, the most critical parameter in the controller tuning, was the selection of the weighting on inputs. During the first half of the simulation, 200 sampling time (100 min) we kept the weights constant at some suitable value, after that as the rate of polymerization increases time varying weights were applied and

once critical conversion is reached again the weights were kept at a constant value as given in equation 6.1 (AMPC Stochastic-without filtering). Fig. 6.4 shows the controlled temperature and corresponding manipulated variable profile under AMPC case. The variation of the coefficients of $A(q)$ and $B(q)$ polynomials and forgetting factor (μ) is shown in Fig. 6.5.

| <i>Parameter</i> | <i>Deterministic</i> | <i>Stochastic (no-filtering)</i> | <i>Stochastic (filtering)</i> |
|--------------------------------------|----------------------|--------------------------------------|-----------------------------------|
| Number of step response coefficients | 95 | 95 | 95 |
| Sampling period, T_s | 30 (sec) | 30 (sec) | 30 (sec) |
| Control horizon, M | 1 | 1 | 1 |
| Prediction horizon, P | 10 | 10 | 10 |
| Weight on input variables, λ | [0.4 0.1] | [0.5 0.1] | [0.5 0.1] |
| Constraints on input | [0 10] | [0 10] | [0 10] |
| Constraints on output | [0 55] | [0 55] | [0 55] |
| Value of parameter α | 0.921 | 0.921 | 0.920 |
| tfilter | [0 ; 9] | [0 ; 9] | [6 ; 9] |

Table 6.1: FMPC design and tuning parameters

| <i>Parameter</i> | <i>Deterministic</i> | <i>Stochastic (no-filtering)</i> | <i>Stochastic (filtering)</i> |
|--------------------------------------|----------------------|--------------------------------------|-----------------------------------|
| Number of step response coefficients | 25 | 25 | 25 |
| Sampling period, T_s | 30 (sec) | 30 (sec) | 30 (sec) |
| Control horizon, M | 1 | 1 | 1 |
| Prediction horizon, P | 24 | 24 | 24 |
| Constraints on input | [0 10] | [0 10] | [0 10] |
| Constraints on output | [0 55] | [0 55] | [0 55] |
| Set point | 55 | 55 | 55 |
| t_{filter} | [0 ; 5] | [0 ; 5] | [5 ; 5] |

Table 6.2: AMPC design and tuning parameters

As we can see from the Figures 6.3 and 6.4 that both controllers, FMPC and AMPC, are tuned to a good performance. We also conclude that AMPC performs better than FMPC.

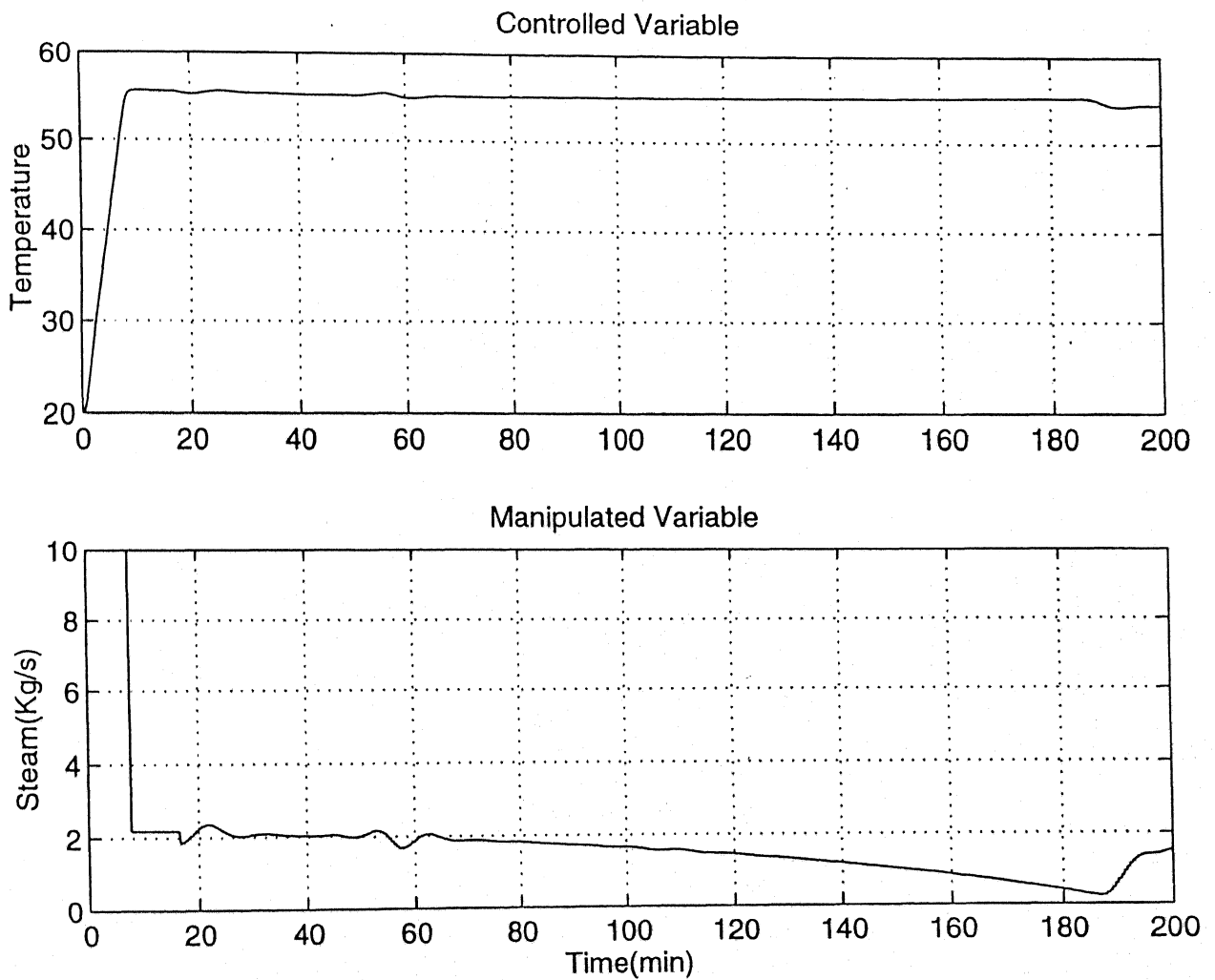


Fig. 6.3: Reactor temperature and manipulated variable

Case: FMPC - deterministic.

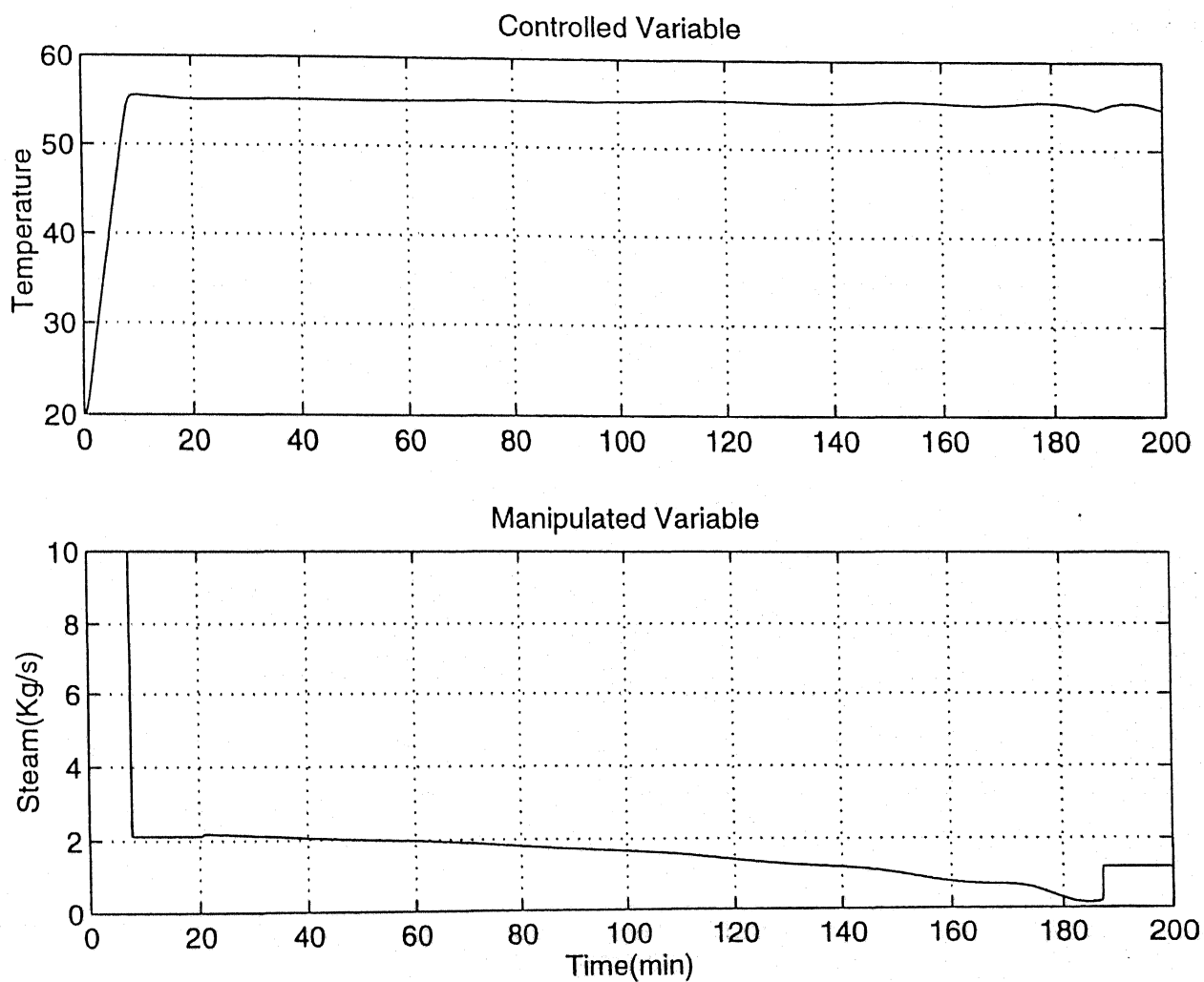


Fig. 6.4: Reactor temperature and manipulated variable

Case: AMPC - deterministic.

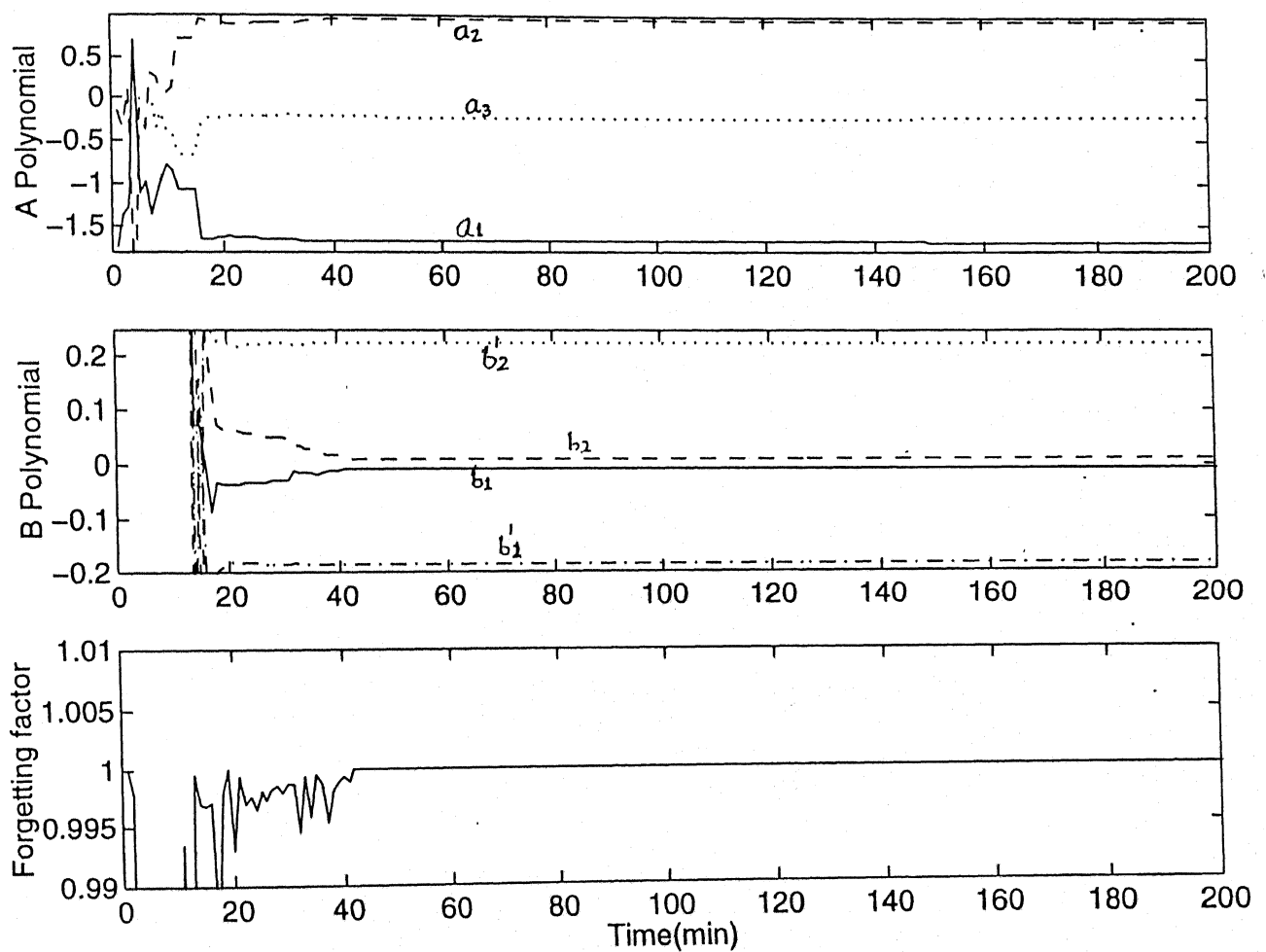


Fig. 6.5: Coefficients of $A(q)$ and $B(q)$ polynomial

Case: AMPC - deterministic.

6.1.3 Stochastic - without filtering

- **FMPC:** In the stochastic case (white Gaussian noise of standard deviation 0.4 added to the temperature measurement), Figure 6.6 shows the performance of the controller. It is clear from the figure that the controller actions are much more aggressive in this case. All the MPC parameters are same as in deterministic case except, the value of input weighting on u_1 and u_2 . FMPC parameters are listed in Table 6.1.
- **AMPC:** In stochastic case it turns out that adaptive MPC is more sensitive to the noise and this can be seen from the plots that FMPC outperforms AMPC. This is due to the poor identification of the process in presence of noise which can be seen by comparing the coefficients of the process transfer function (Figure 6.8) with those in the deterministic case (Figure 6.5). In stochastic case the variation of parameters is irregular. The design parameters of AMPC are the same as in deterministic case (Table 6.2). Selection of input weights was of prime importance and it has been done like this:

1. For 1 - 200 samples, Input weight (λ) = [0.48 0.20]
2. For 200 - 340 samples, $\lambda(k+1) = \lambda(k) - [0.0018 \ -0.00021]$
3. For 340 - 400 samples, $\lambda = [0.17 \ 0.21]$ (6.1)

where,

first column of λ - weight on u_1 .

second column of λ - weight on u_2 .

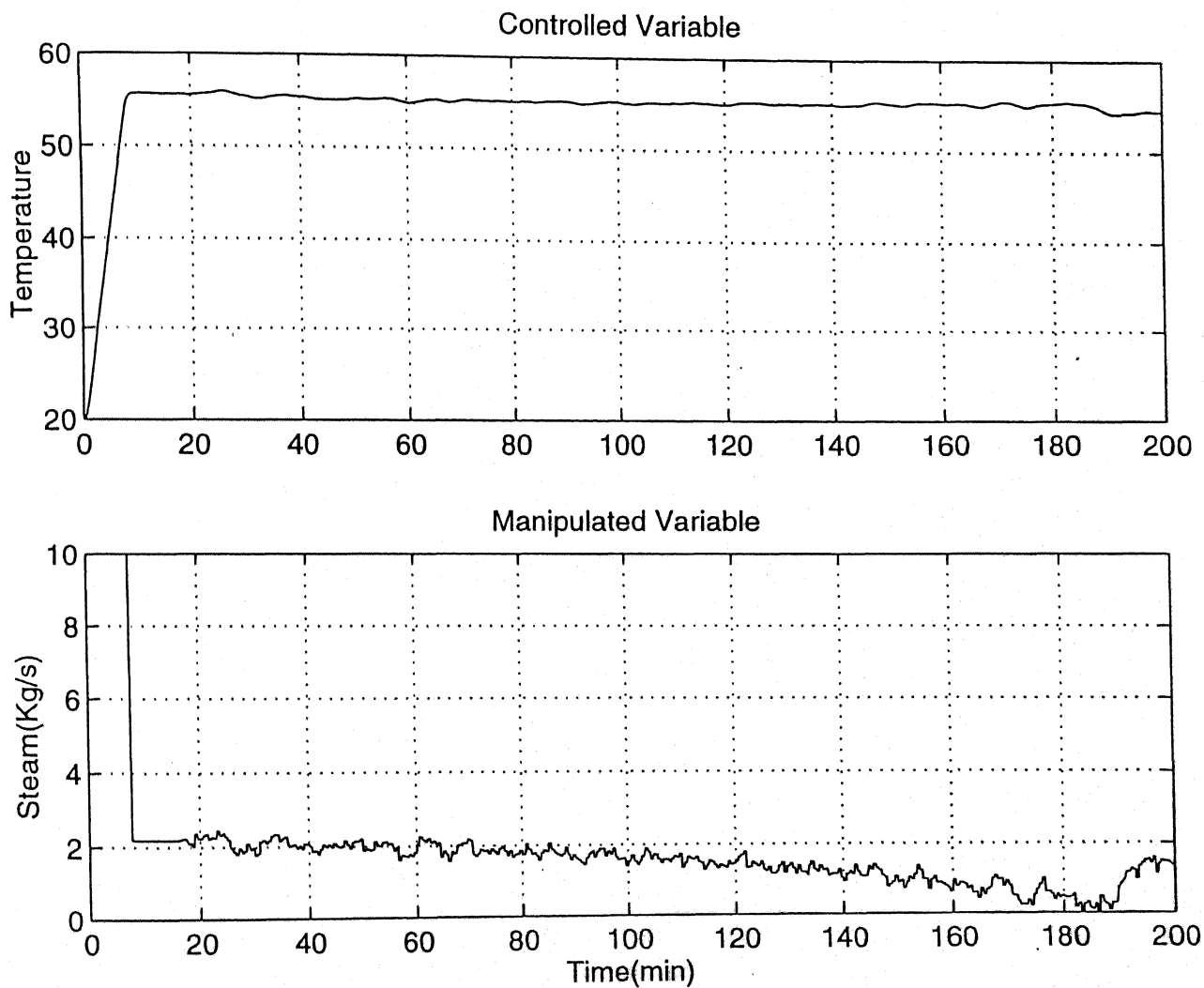


Fig. 6.6: Reactor temperature and manipulated variable

Case: FMPC - Stochastic (without filtering).

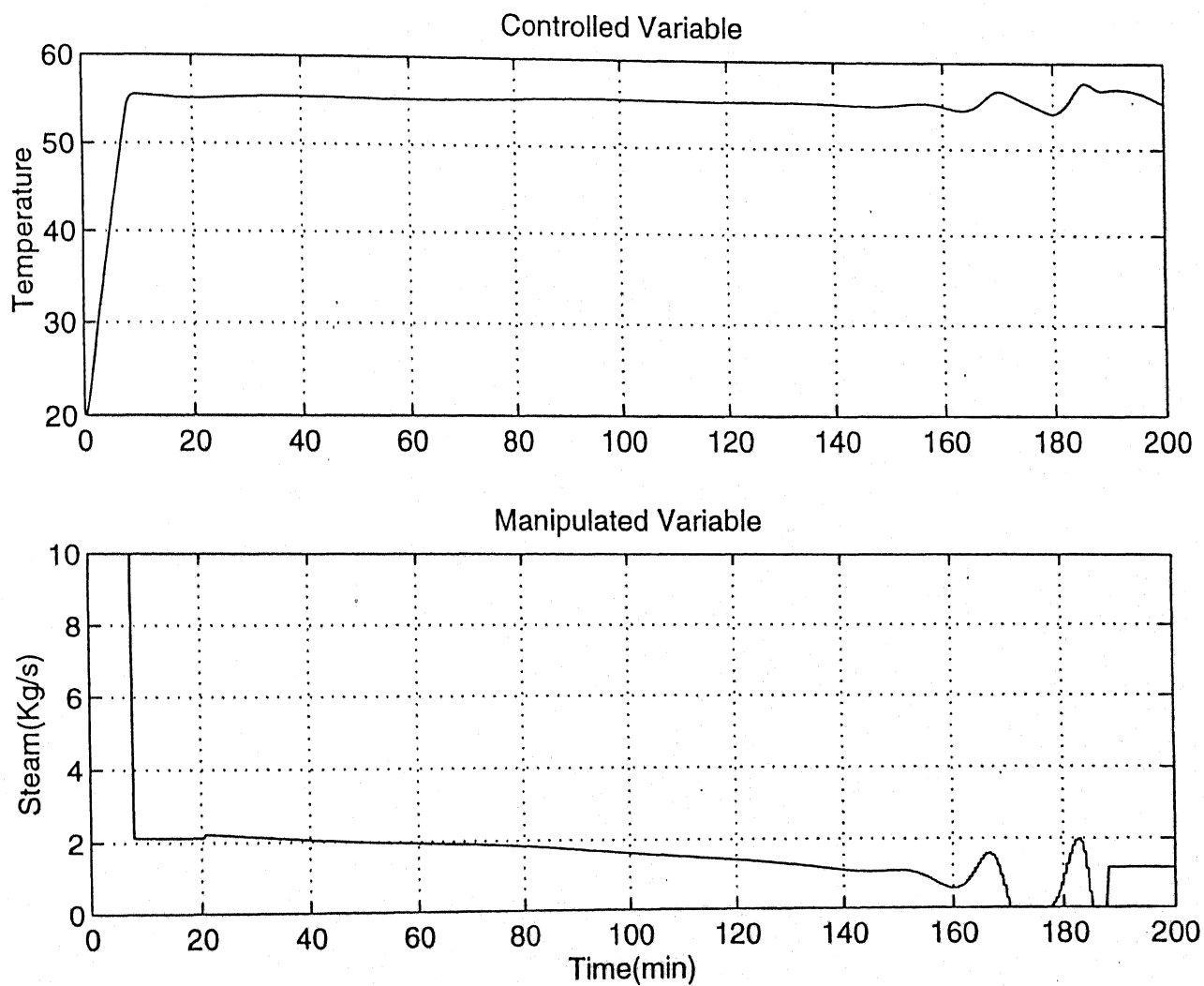


Fig. 6.7: Reactor temperature and manipulated variable

Case: AMPC - Stochastic(without filtering).

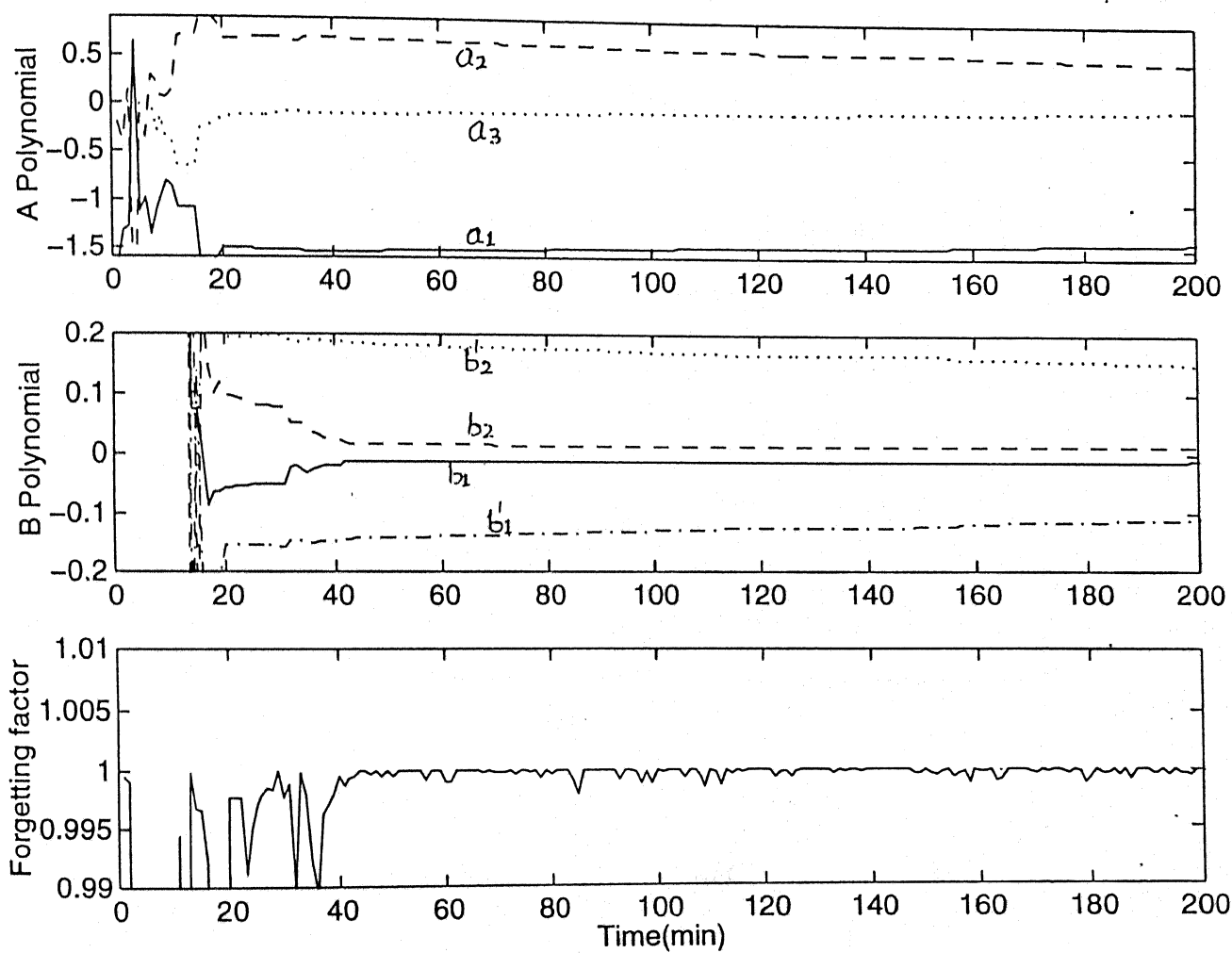


Fig. 6.8: Coefficients of $A(q)$ and $B(q)$ polynomial

Case: AMPC - Stochastic(without filtering).

6.1.4 Stochastic - with filtering

- **FMPC:** Now we consider the case where the noisy temperature measurement is passed through an analog filter (a first order system). The time constant of the noise filter was chosen to be 6 sec. Reactor temperature is plotted in Figure 6.9. There is significant improvement in the performance of FMPC and it is nearly as good as in the deterministic case (Figure 6.3). The design parameters of FMPC are again the same except one change in set point parameter α (Table 6.1).
- **AMPC:** For this case if we compare the performance of AMPC (Figure 6.10) with FMPC (Figure 6.9) it turns out that both AMPC & FMPC performs very well in maintaining the constant temperature profile (Table 6.3). Time constant for noise filter has been chosen as 5 sec (Table 6.2). The variation of plant coefficients is shown in Figure 6.11. Here again the variation in plant coefficients as well in forgetting factor is more significant.

| Table 6.3: Comparison of results | | |
|----------------------------------|------------|--------|
| Case | Controller | CRE |
| Deterministic | FMPC | 0.5216 |
| | AMPC | 0.4562 |
| Stochastic(without filter) | FMPC | 0.7650 |
| | AMPC | 1.0426 |
| Stochastic(with filter) | FMPC | 0.6361 |
| | AMPC | 0.5720 |

In table 6.3 the criteria used for the comparison is maximum error (CRE) which usually occurs around the critical conversion. This error is calculated as :

$$\text{CRE} = \max(y - w) \text{ after the } n\text{th sample.}$$

where

- y = actual output of the system (temperature).
- w = set point value.
- n is the earliest sample at which $y = w$.

If we compare the results on the basis of the error calculated in the Table 6.3, it is clear that AMPC performs better than FMPC in deterministic and stochastic - with filtering cases while FMPC outperforms in the second case (stochastic - without filtering). Overall both the schemes were found to be successful in controlling the temperature of the PVC reactor at a constant value of 55 °C.

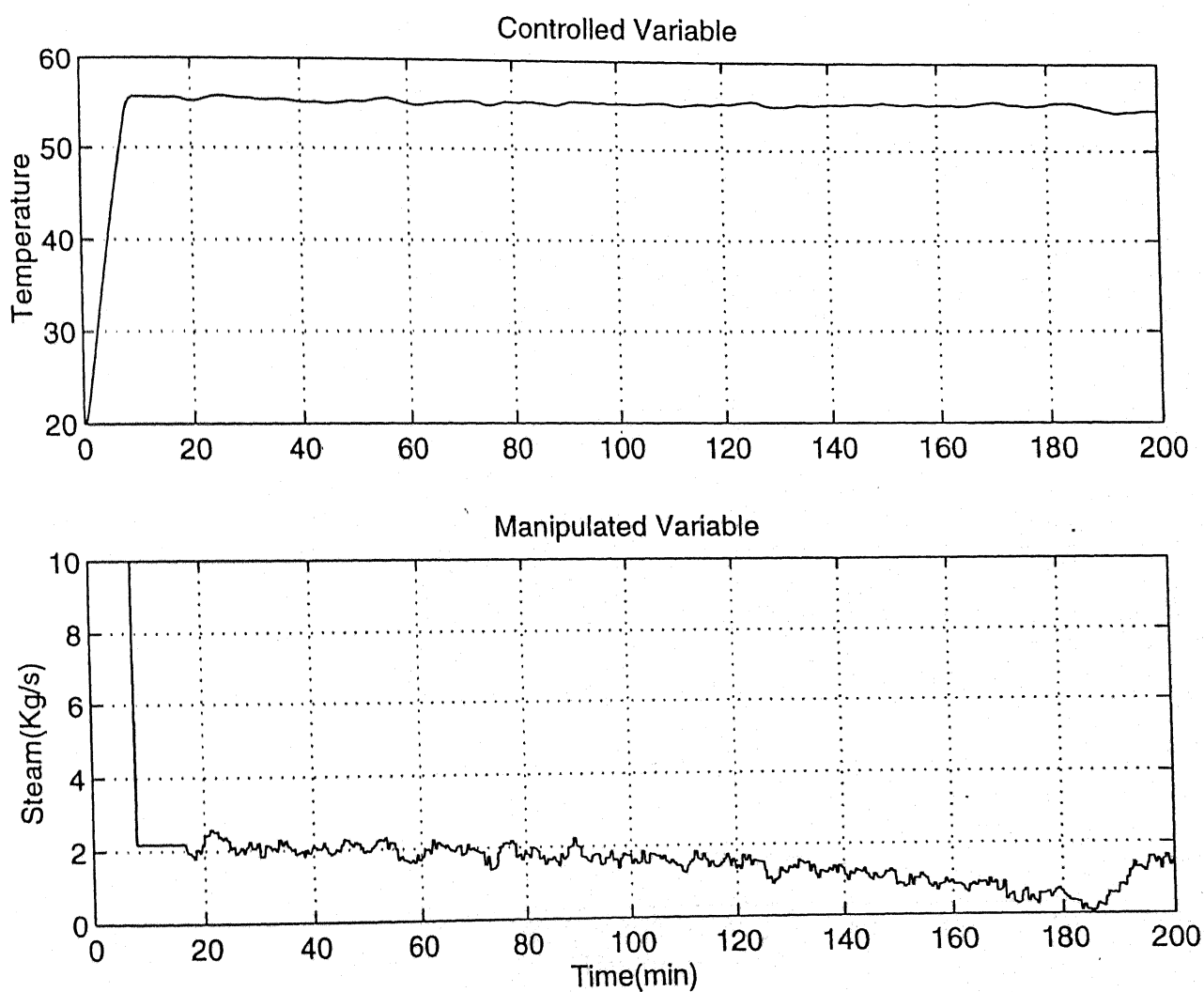


Fig. 6.9: Reactor temperature and manipulated variable

Case: FMPC - Stochastic(with filtering).

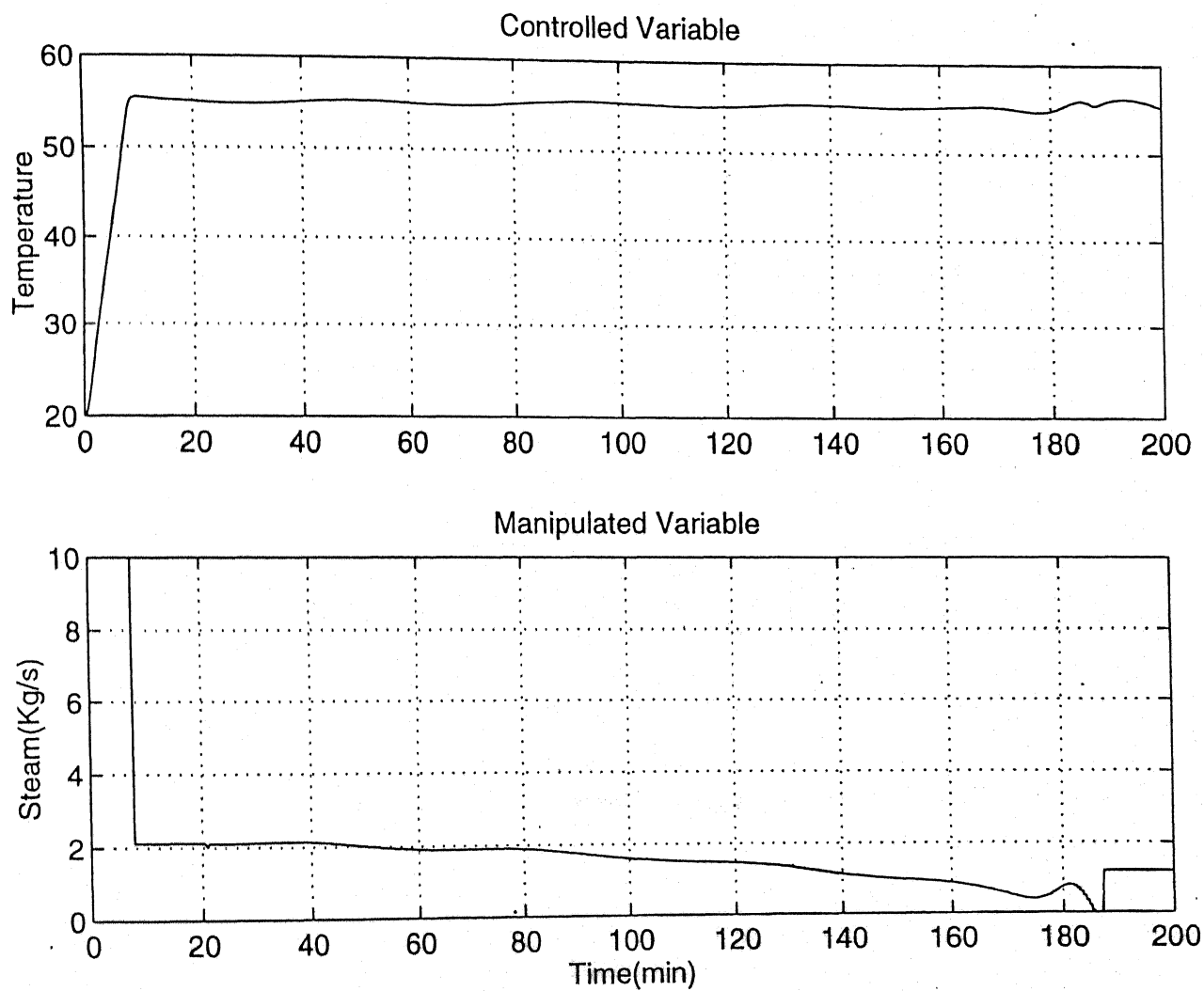


Fig. 6.10: Reactor temperature and manipulated variable

Case: AMPC - Stochastic (with filtering).

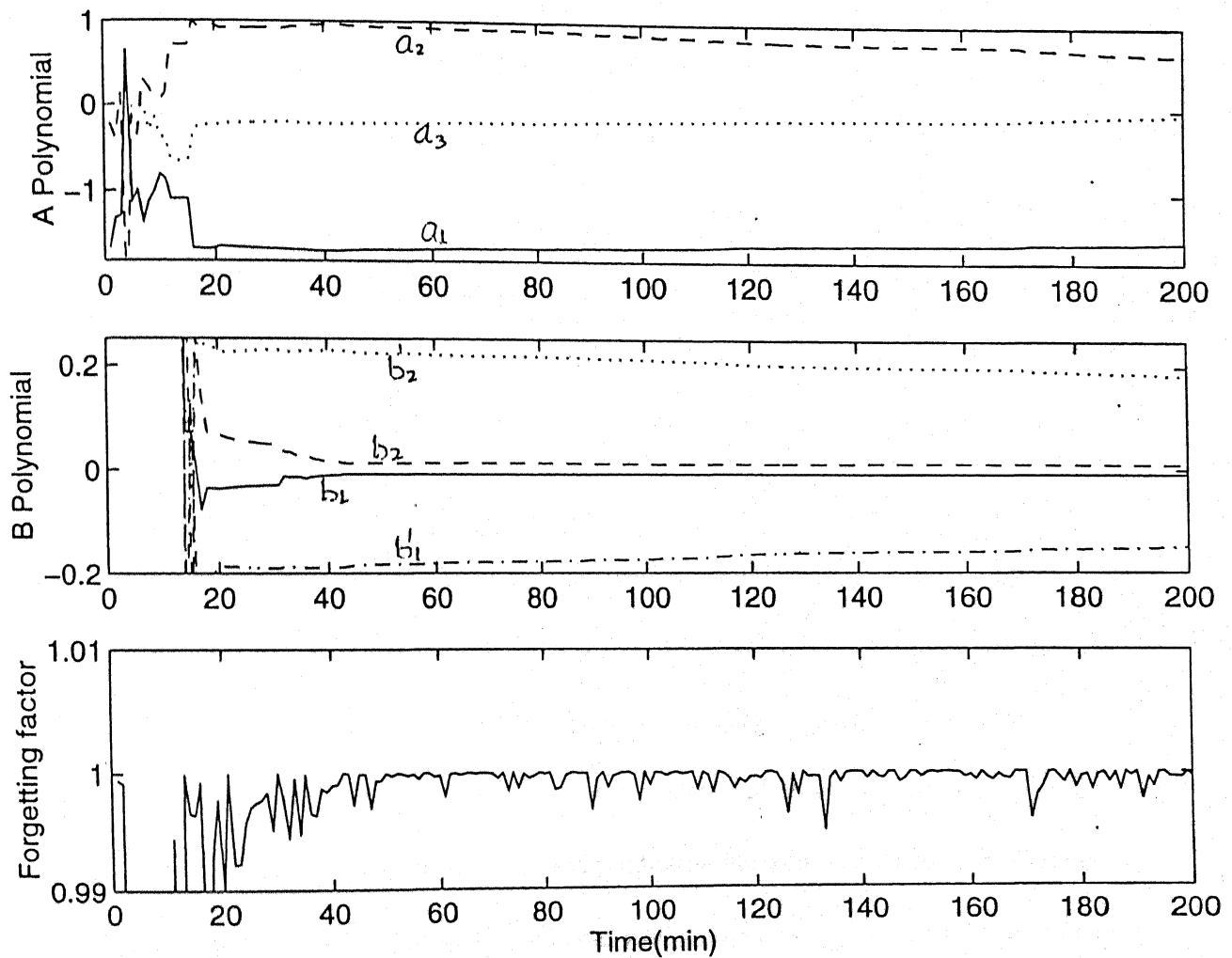


Fig. 6.11: Coefficients of $A(q)$ and $B(q)$ polynomial

Case: AMPC - Stochastic (with filtering).

6.2 Molecular Weight Control

In this section we discuss the control results when our objective is to achieve the desired molecular weight of PVC. First we present the step response model of the process and then the simulation results obtained.

6.2.1 Step response model

For this case, as there is no scheme available for the identification of a MIMO system so we developed two SISO models and then these two models have been appended to form a composite model that retains the inputs and outputs of the original models. First model has been developed using steam as an input and M_w as output variable while second model is based on cold water as an input and M_n as output. Figure 6.12 shows the step response of u_1 (steam) to the outputs M_w and M_n and Figure 6.13 shows the step response of u_2 (cold water) to the same outputs.

6.2.2 Simulation results of FMPC

Figure 6.14 shows the molecular weight (weight average and number average) profile under isothermal control of reactor. Then we have attempted to control the molecular weight with steam as manipulated variable and with a sampling time of 5 minutes. The MPC design parameters were selected after several simulation trials. The control horizon was chosen as $M=5$, and prediction horizon was $P=20$. Input weights (λ) were set to 0.1 and 0.3 for steam and cold water respectively. Detailed parameter values are listed in Table 6.4. Figure 6.15 shows the performance obtained using the FMPC with a set point of 70000 for M_w and 35000 for M_n . It can be seen from the results that the desired molecular weights have been achieved at the end of the reaction. In Figure 6.16 the distribution of the Polydispersity Index (PDI) with time has been

presented. PDI of the polymer varies between 2 and 2.4, and at the end it approaches a value of 2.35.

Table 6.4: FMPC design and tuning parameters
Case : Molecular Weight Control

| | |
|--------------------------------------|-----------|
| Number of step response coefficients | 10 |
| Sampling period, T_s | 5 (min) |
| Control horizon, M | 5 |
| Prediction horizon, P | 20 |
| Weights on input, λ | [0.1 0.3] |
| Constraints on input (u_1) | [0 10] |
| Constraints on output, M_w | [0 70000] |
| Constraints on output, M_n | [0 35000] |
| Set point for M_w | [70000] |
| Set point for M_n | [35000] |

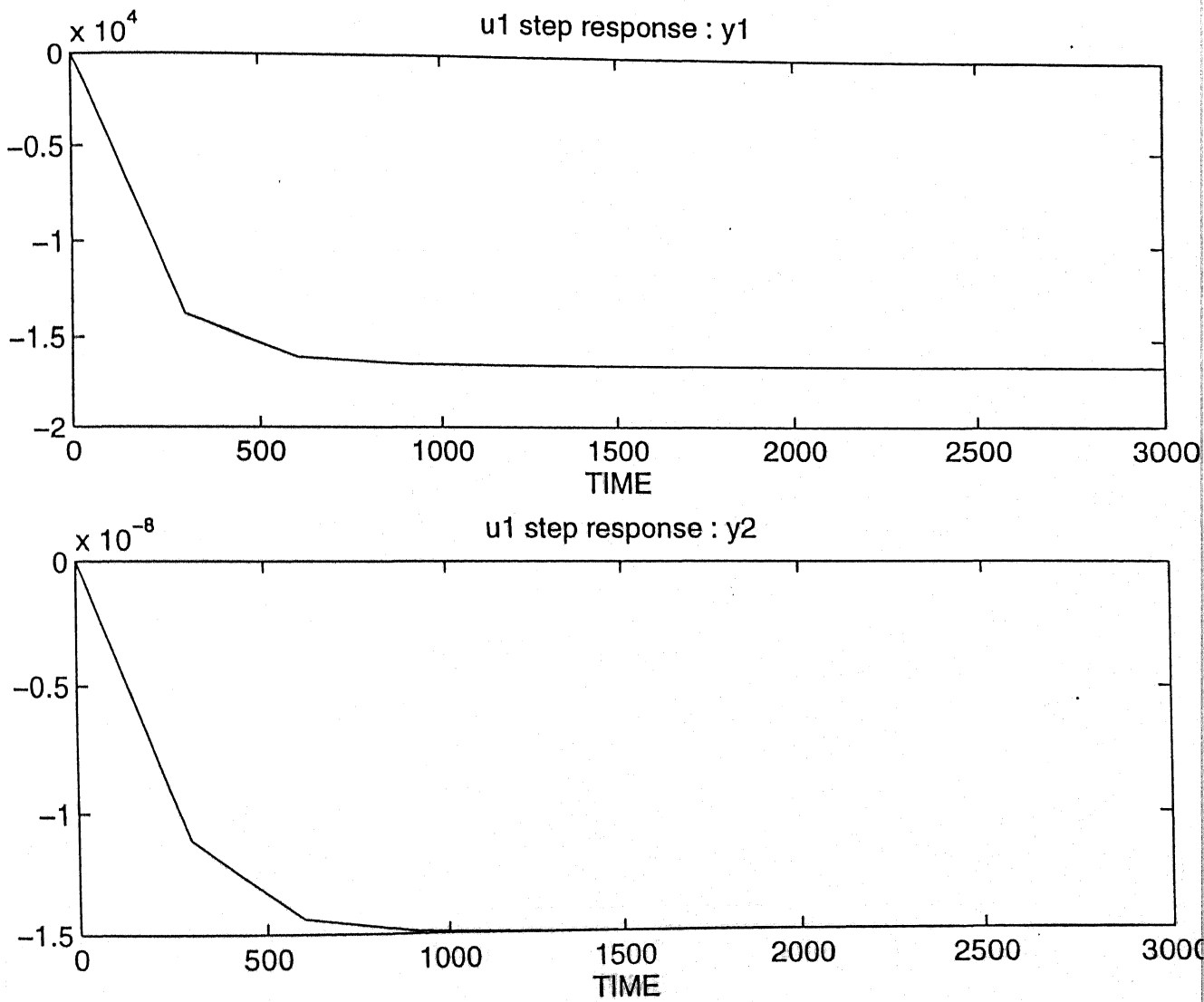


Fig. 6.12: Plot of step response, u_1 - steam flow rate.

$y_1 - M_w$; $y_2 - M_n$

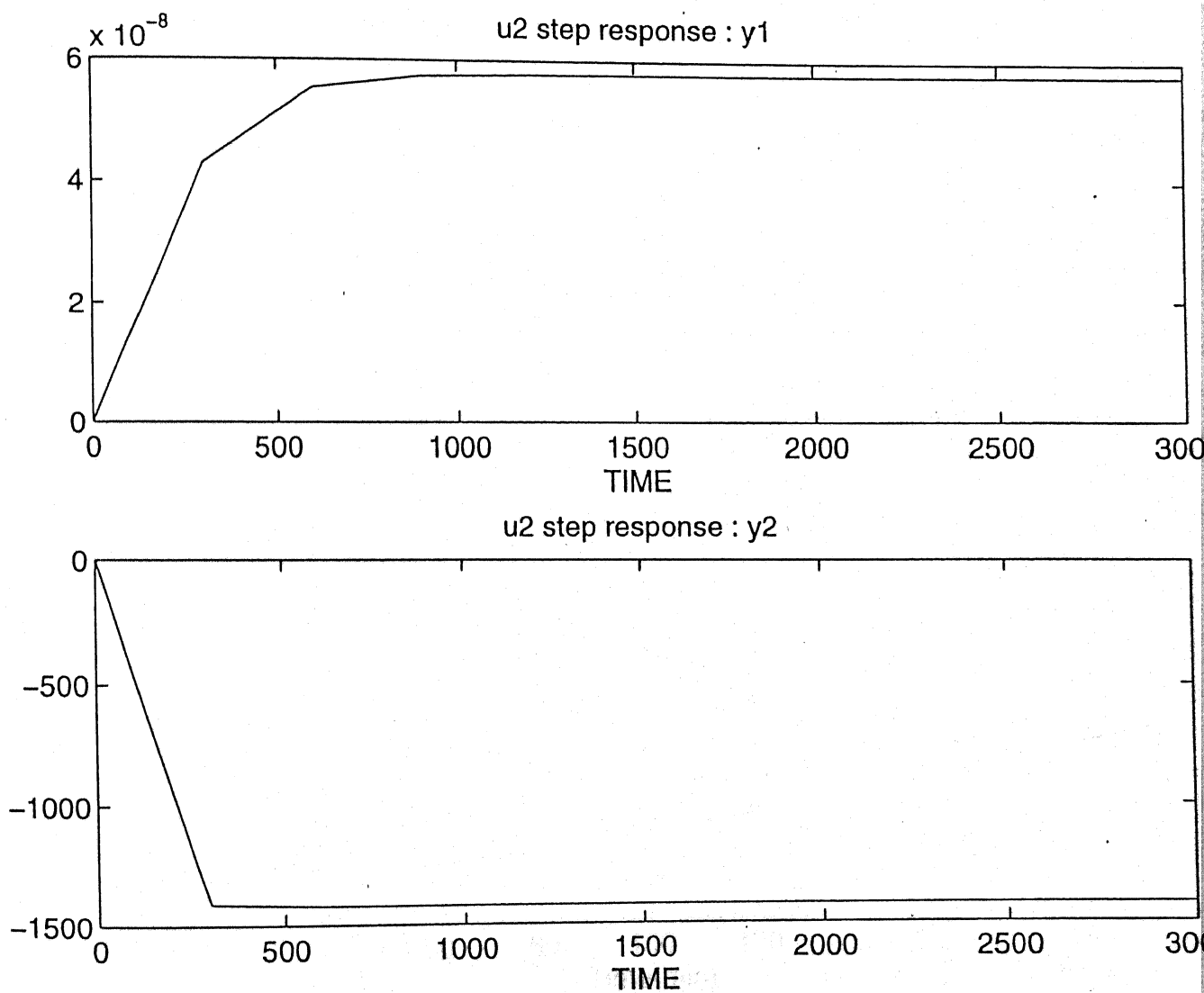


Fig. 6.13: Plot of step response, u_2 - cold water

$y_1 - M_w$; $y_2 - M_n$ Molecular weight distribution - under isothermal control

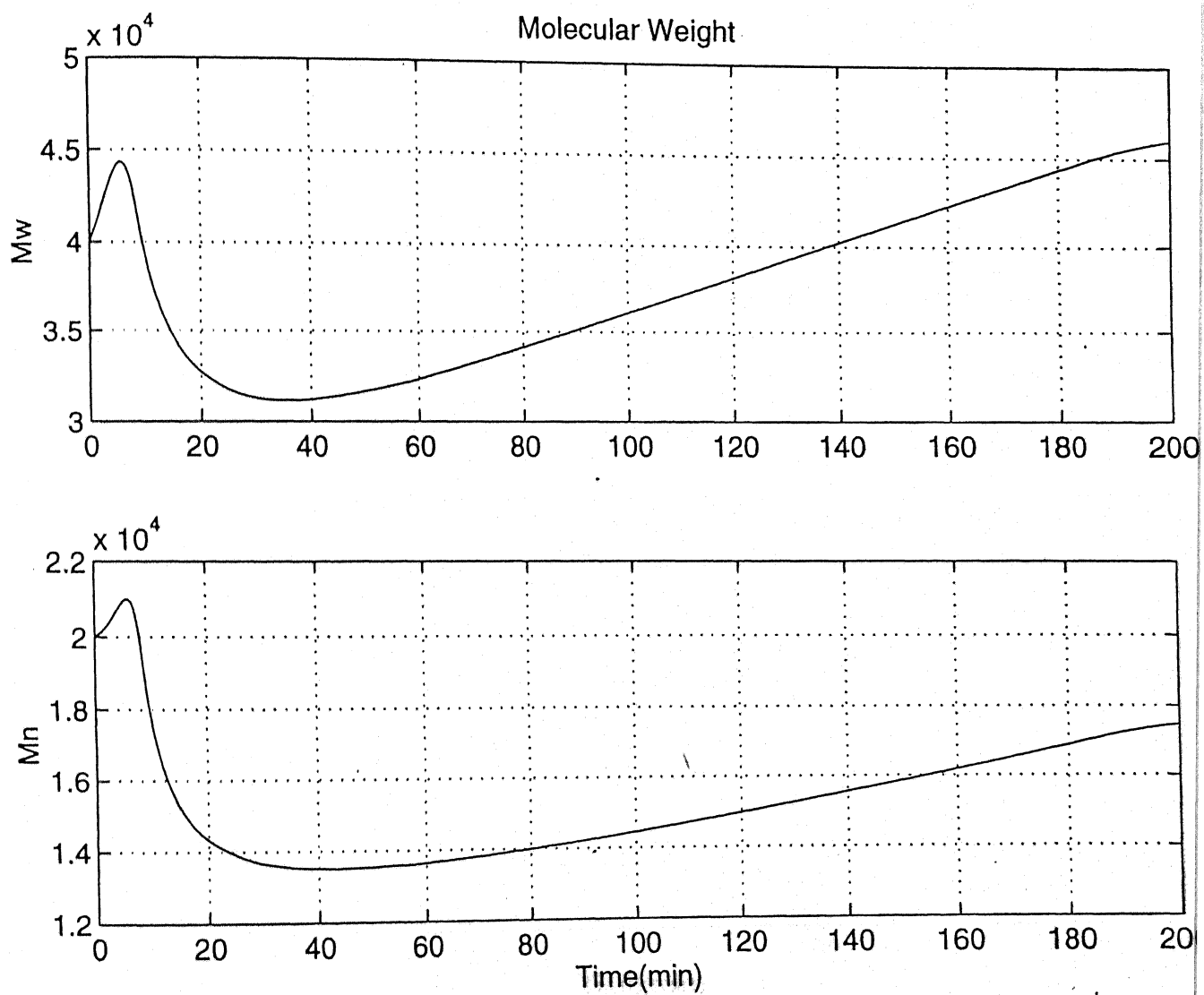


Fig. 6.14: Average Molecular weight distribution - under isothermal control.

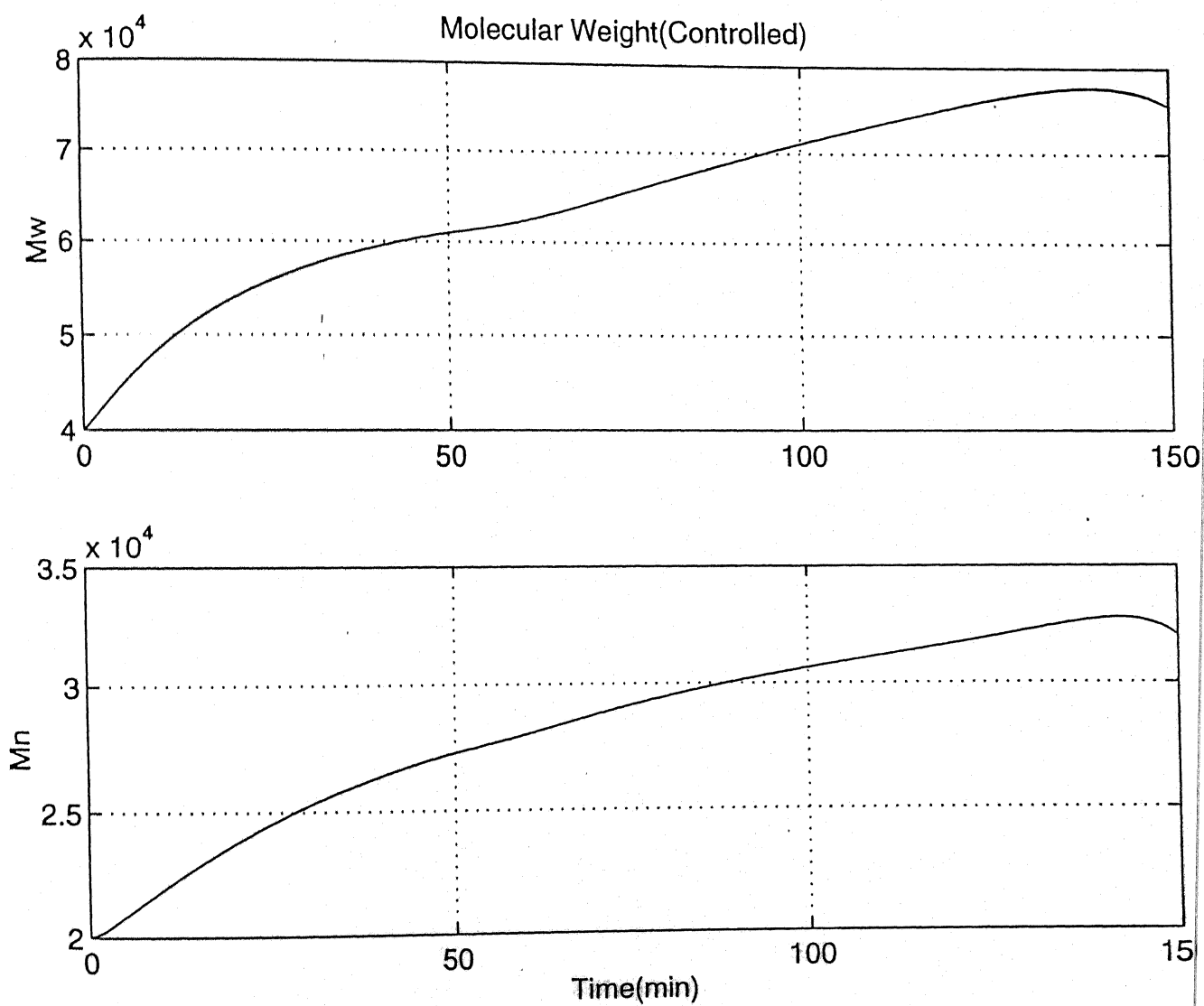


Fig. 6.15: Average molecular weight distribution - Controlled

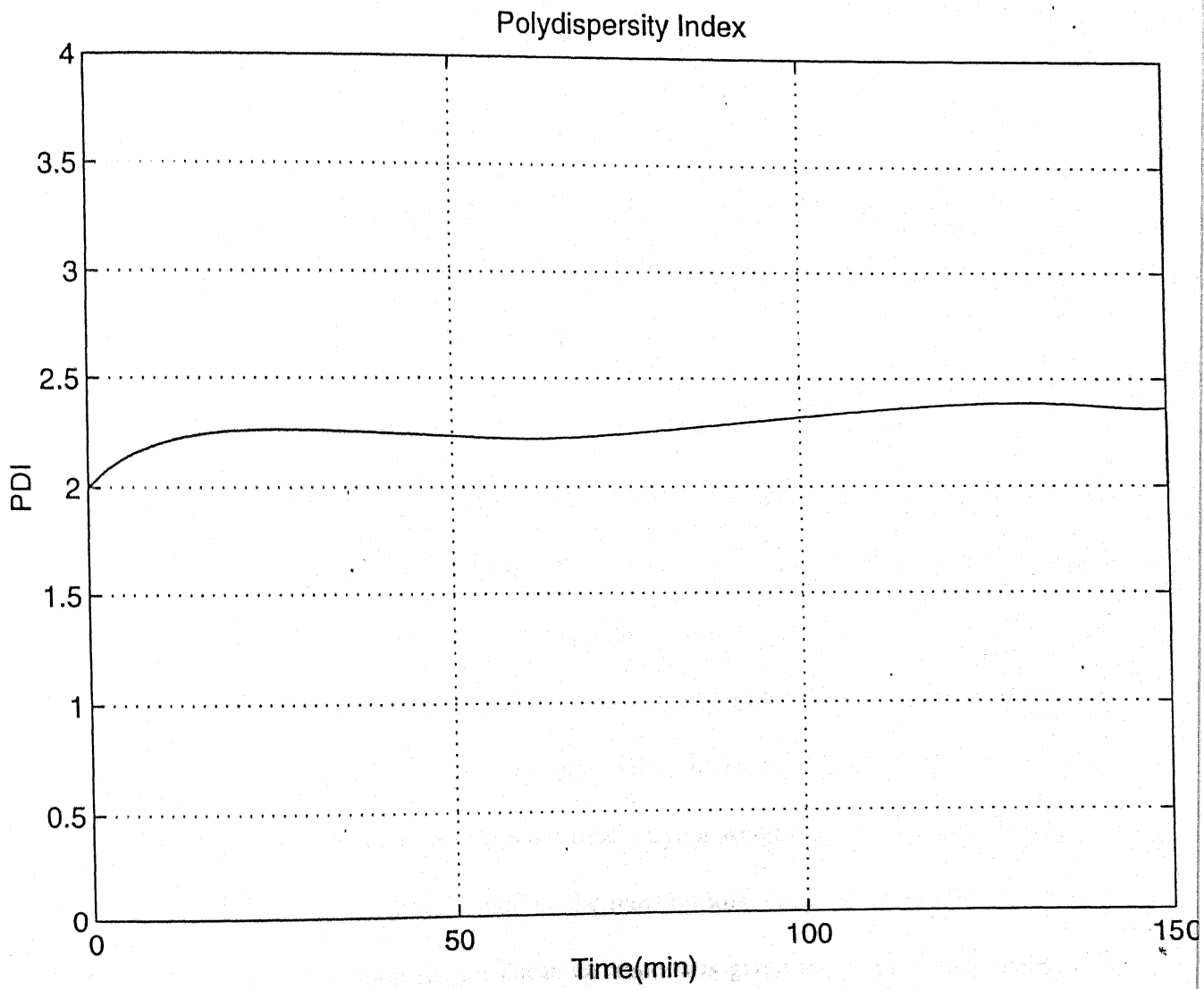


Fig. 6.16: Plot of Polydispersity Index (PDI).

Chapter 7

Conclusions and Recommendations

We have presented a control system design (MPC) in its two forms FMPC and AMPC to control a batch reactor. It has been found that it performs better than other controllers that were used for this system. Performance of MPC was found to be comparable to that of GPC (Ritwik Bhatia, 1996). The simulation results show that MPC in its fixed form was robust enough to be used without on-line adaptation of the model parameters even though the system was time varying.

The most important part of the MPC control was found to be the tuning of the controller. We started with some tuning guidelines available in the literature and after several simulation runs we could come to the final selection of the parameters. Apart from the control horizon (M) and prediction horizon (P) the most crucial design parameter was weight on input variables. After several trials it turned out that FMPC can perform well with constant input weights while in the case of AMPC, where model parameters changes every sample time, time varying weights made it more robust. We kept the weights constant up-to half of the reaction time (200 samples) and after which as rate of polymerization rises a linear variation was given to weights and finally after critical conversion the weights were again kept at a constant value. This strategy turned out to be very effective.

Noise filter was used to attenuate the effect of noise. It significantly improved the performance of adaptive MPC.

Molecular weight is one of the desired property of any polymer. We apply the MPC control algorithm to control the molecular weight of the PVC subjected to constraints, and get the desired molecular weight and polydispersity at the end of the reaction. From the results we see that it has been possible to achieve the $M_w \cong 70000$, and $M_n \cong 35000$ with a polydispersity value of around 2.35.

The recommendations for the further work are -

1. The inaccurate identification of the plant in presence of noise caused adaptive MPC to perform relatively poorly and was not able to handle the noise of that level which FMPC did. It is a therefore important that algorithms that overcome this problem be worked out.
2. Another proposal for further work is that one cascade control system can be developed in which there will be two MPC controllers, inner for temperature control and outer for the molecular weight control. In inner controller, steam will be output variable and temperature will be the input variable with a sampling time of 30 sec. In outer controller molecular weight, will be passed as an input and temperature will be the output variable which will be passed as a set point for the inner controller after every 5/10 minutes (sampling time for this system).

Appendix A

A.1 Calculation of y^{past} , d^{ext} and A

By definition, the vector y^{past} is the output at each sampling time in the future with all the future input changes set equal to zero. In the linear MPC, y^{past} is calculated from the first two terms in eqn. (3.3) based on the past inputs only. The nonlinear equivalent of y^{past} is to integrate the nonlinear state equations $\dot{x} = f(x, u)$ forward from an initial condition of the current modeled states, $x^m(k)$, with a constant input, $u = u(k-1)$, over the future horizon P (Garcia, 1984). Next the output is reconstructed from the integrated states using the algebraic output equation $y = g(x)$.

The disturbance effect, d^{ext} is estimated similar to the linear MPC except that instead of the linear model in Fig. (3.3) a nonlinear model is simulated in parallel to the plant. The state is integrated from its initial value (one sampling time ago), $x(k-1)$, to the present value, $x^m(k)$, using the past, known value of the control input. The effects of the past inputs on the current output and the current disturbance estimate can then be calculated from

$$y^m(k) = g[x^m(t)] \quad (\text{A.1})$$

$$d^{\text{ext}}(k) = y^{\text{meas}}(k) - y^m(k) \quad (\text{A.2})$$

Like in linear MPC, d^{ext} is assumed to remain constant over the prediction horizon P. When a perfect nonlinear model is used, d^{ext} is due to external disturbances only and does not contain model/plant mismatch due to linear approximation. If the

nonlinear model is not perfectly known, \mathbf{d}^{ext} will contain modeling errors in addition to external process disturbances.

The dynamic matrix \mathbf{A} or the step- response coefficients are calculated either from the linear model obtained after linearizing the nonlinear model at a given steady state or by perturbing the nonlinear dynamic model by a unit step.

A.2 Stability

The stability of the closed-loop system can be characterized by using contraction mapping ideas. We look at the nonlinear operator \mathbf{N}

$$\begin{bmatrix} \mathbf{x}_{k+1} \\ \mathbf{u}_{k+1} \end{bmatrix} = \mathbf{N} \begin{bmatrix} \mathbf{x}_k \\ \mathbf{u}_k \end{bmatrix}$$

where k denotes the sampling time. The closed- loop system is stable if the norm of the gradient of \mathbf{N} is less than one for all (\mathbf{x}, \mathbf{u}) in a closed convex set S , where $\mathbf{N}: S \rightarrow S$.

The following theorem gives sufficient conditions for stability. Even though the theorem's applicability may be limited, it does yield valuable understanding of the effect of various parameters on the closed-loop stability of the control algorithm.

Theorem : Suppose that the system to be controlled is globally asymptotically stable for all feasible inputs. Furthermore, suppose that the following is valid:

1. The steady - state gain of the system does not change sign.
2. The weight on the change of the input is larger than zero.
3. The sampling time is "long enough" .
4. The input horizon M is set to one .

5. The set point is constant in the prediction horizon.

Then the closed-loop system is guaranteed to be nominally stable.

Appendix B

Recursive Identification Algorithm

It is assumed that the plant is described by the discrete time relationship

$$A(q)y(t) = B(q)u(t-1) + T(q)\xi \quad (\text{B.1})$$

where, $A(q)$ and $B(q)$ are polynomials in the backward shift operator (q^{-1}). The form of these polynomials is

- $A(q) = 1 + a_1q^{-1} + a_2q^{-2} + \dots + a_{na}q^{-na}$
- $B(q) = b_1 + b_2q^{-1} + \dots + b_{nb}q^{-nb+1}$
- $T(q) = 1 + t_1q^{-1} + t_2q^{-2} + \dots + t_{nt}q^{-nt}$
- ξ is white noise.

eqn B.1 can be written compactly as

$$\hat{y}(t) = \phi^T(t-1)\theta \quad (\text{B.2})$$

where,

- $\phi^T(t) = [-y(t), \dots, -y(t - na + 1), u(t-1), \dots, u(t - nb)]$
- $\theta(t) = [a_1, \dots, a_{na}, b_1, \dots, b_{nb+1}]^T$

The objective of the identification algorithm is to estimate the current parameter vector $\theta(t)$ such that the function V_t is minimized

$$V_t = \sum_{i=1}^t \alpha(t) [y(t) - \phi^T(t-1) \hat{\theta}(t-1)]^2 \quad (\text{B.3})$$

where, $\alpha(t)$ is a weighting factor. In the RLS with constant forgetting factor, older data is given exponentially less weight, i.e. $\alpha(t) = \mu^{t-i}$. Here μ is called the forgetting factor and is a constant. The objective function is

$$V_t = \sum_{i=1}^t \mu^{t-i} [y(t) - \phi^T(t-1) \hat{\theta}(t-1)]^2 \quad (\text{B.4})$$

In the variable forgetting factor algorithm (Fortescue, 1981) the forgetting factor is not kept constant but varies with time. $\mu(t)$ is calculated in such a manner that the weighted sum of a posteriori errors (Σ_t) is kept a constant value (Σ_0).

$$\Sigma_t = \sum_{j=1}^t (\mu(t))^{t-j} [y(t) - \phi^T(t-1) \hat{\theta}(t)]^2 \quad (\text{B.5})$$

The recursive least squares (RLS) algorithm with variable forgetting factor proposed in (Fortescue, 1981) results from eqn B.1, eqn B.4 and eqn B.5. The algorithm is stated below

1. Prediction $\hat{y}(t) = \phi^T(t-1) \hat{\theta}(t-1)$
2. Error $\varepsilon(t) = y(t) - \hat{y}(t)$
3. Gain $K(t) = P(t-1) \phi(t-1) / [1 + \phi^T(t-1) P(t-1) \phi(t-1)]$
4. Estimates $\hat{\theta}(t) = \hat{\theta}(t-1) + K(t) \varepsilon(t)$
5. Forgetting $\mu(t) = 1 - [1 - \phi^T(t-1) K(t)] \varepsilon(t)^2 / \Sigma_0$
6. Covariance $P(t) = [1 - K(t) \phi^T(t-1)] P(t-1) / \mu(t)$

Appendix C

Computer programs

C.1 Nonlinear Adaptive MPC

```
function [sys,x0] = nlmpcsim(t,x,sysu,flag,modelpd,Kmpc,r,usat,tfilter,ud0)

%
%NLMPCSIM S-function for SIMULINK block nlmpcsim.
% Usage:  [sys,x0] = nlmpcsim(t,x,sysu,flag,modelpd,Kmpc,r,usat,tfilter,ud0);
%
% Masked inputs (required):
%  modelpd: =[model dmodel], step response model for plant and disturbance in Step
Format.
%  Kmpc: MPC controller gain generated by mpcccon.
%  r:   a constant or time-varying reference trajectory.
%  usat: matrix of manipulated variable constraints. Default=[].
%  tfilter: time constants for noise filter and unmeasured disturbance lags.
%          Default is no filtering and step disturbance.
%  ud0: =[u0 d0] initial conditions for manipulated variables (u) and measured
disturbances.
% Determine system size
```

% nu: number of inputs to the plant (= outputs from the MPC controller)

% ny: number of outputs from the plant

% nd: number of measured disturbances

global Kmpc tsamp modelpd

global Nident na nb nk z Uident Yident

global th p phi A B thm mod

global fd currSamp adm ff

global tfinal delt2 M P uwt ywt ulim ylim usat tfilter y0 u0 d0 ud0 r

if flag == 0

file = 'x';

[fd message] = fopen(file,'wt');

if fd == -1

error(message);

end

na= 3 ;

nb= [2 2];

nk= [1 1];

load data

extract;

y=y3(1:20);

u=[u1(1:20) u2(1:20)];

z=[y u];

z=dtrend(z);

Yident = y ; Uident = u;

```

Nident=[na nb nk];

adm = 'fv';

ff = 1.0;

[th,yh,p,phi,lam] = rarx_vff(z(1,:),Nident,adm,ff);

for k = 2:20

    [th,yh,p,phi,lam] = rarx_vff(z(k,:),Nident,adm,ff,th',p,phi);

end

A = zeros(1,na+1); A(1) = 1.0;

B = zeros(1,1:nb(1)+nk(1));

B = zeros(2,1:nb(2)+nk(2));

% A(1)=1;

% A(2:na+1) = th(1:na);

% B(1,1:nk(1)) = zeros(1,nk(1))

% B(1,nk(1)+1:nb(1)+nk(1)) = th(na+1:na+nb(1))

% B(1,nk(1)+1:nb(1)+nk(1)) = th(na+1:na+nb(1))

% B(2,1:nk(2)) = zeros(1,nk(2));

% B(2,nk(2)+1:nb(2)+nk(2)) = th(na+nb(1)+1:na+nb(1)+nb(2));

% thm = poly2th(A,B)


thm = arx_id(z,Nident);

mod = th2mod(thm);

tfinal=750;

delt2= 30;

[model,dmodel]= mod2step(mod,tfinal,delt2);

```

```

modelpd = [model dmodel];

mpcpara_on;           % file containing parameters

uwt= [0.48 0.20];

tfilter= [0 ; 5];

Kmpc= mpcccon(model,ywt,uwt,M,P);


[nrow,nund] = size(modelpd);

ny = modelpd(nrow-1,1);

for i = 2:nund,

    if modelpd(nrow-1,i) ~= 0 & modelpd(nrow-1,i) == ny,

        nd = nund-i+1;

    elseif modelpd(nrow-1,i) ~= 0 & modelpd(nrow-1,i) ~= ny,

        error('Number of outputs for model and dmodel must be the same')

        return

    else

        nd = 0;

    end

end

nu = nund - nd;

model = modelpd(:,1:nu);

dmodel = modelpd(:,nu+1:nund);

tsamp = model(nrow,1);

if isempty(ud0),

    ud0 = zeros(1,nund);

```


end

[nrKmpc,ncKmpc] = size(Kmpc);

z = ncKmpc/ny;

sys = [0 nu nu ny+nd 0 0];

x0 = ud0(1:nu);

elseif flag == 3, % The outputs are equal to the states.

 currSamp = round(t/tsamp);

if currSamp <16

 sys(1) = 10;

 sys(2) = 49.75;

elseif currSamp <42

 sys(1) = 2.12;

 sys(2) = 49.75;

elseif currSamp >374

 sys(1) = 1.18;

 sys(2) = 49.75;

else

 sys = x;

end

elseif flag == 4, % Determine the next sampling time.

 sys = tsamp*(1+floor(t/tsamp+1e-12*(1+t/tsamp)));

elseif flag == 2,

```
currSamp = round(t/tsamp)
```

```
sys = x;           % If not at sampling time, states are not changed
```

```
yp = sysu;         % Get the current measurement.
```

```
Yident = yp
```

```
Uident = [sys(1) sys(2)]
```

```
[th,yh,p,phi,lam] = rarx_vff([Yident Uident],Nident,adm,ff,th',p, phi);
```

```
if abs(round(t/tsamp) - t/tsamp) < 1e8*eps
```

```
    A(1)=1; A(2:na+1) = th(1:na);
```

```
    B(1,1:nk(1)) = zeros(1,nk(1));
```

```
    B(2,1:nk(2)) = zeros(1,nk(2));
```

```
    B(1,nk(1)+1:nb(1)+nk(1)) = th(na+1:na+nb(1));
```

```
    B(2,nk(2)+1:nb(2)+nk(2)) = th(na+nb(1)+1:na+nb(1)+nb(2));
```

```
    A;
```

```
    B;
```

```
    if currSamp >= 1
```

```
        for i=1:7,
```

```
            fprintf(fd,'%0.6f ',th(i)); end
```

```
            fprintf(fd,'%e\n' ,lam);
```

```
            if currSamp == 400, fclose(fd); end
```

```
        end
```

```
        thm= poly2th(A,B);
```

```
        mod = th2mod(thm);
```

```

[model,dmodel]= mod2step(mod,tfinal,delt2);

modelpd = [model dmodel];

if currSamp < 200

    uwt = uwt

elseif currSamp < 340

    uwt= uwt - [0.0018 -0.00021]

else

    uwt = [0.17 0.21]

end

Kmpc= mpcccon(model,ywt,uwt,M,P);

end

[nrow,nund] = size(modelpd);

ny = modelpd(nrow-1,1);

for i = 2:nund,

    if modelpd(nrow-1,i) ~= 0 & modelpd(nrow-1,i) == ny,

        nd = nund-i+1;

    elseif modelpd(nrow-1,i) ~= 0 & modelpd(nrow-1,i) ~= ny,

        error('Number of outputs for model and dmodel must be the same')

    return

else

    nd = 0;

end

end

```

```

nu = nund - nd;

model = modelpd(:,1:nu);

dmodel = modelpd(:,nu+1:nund);

tsamp = model(nrow,1);

if isempty(ud0),

    ud0 = zeros(1,nund);

end

[nrKmpc,ncKmpc] = size(Kmpc);

z = ncKmpc/ny;

if t == 0,

    y0 = yp(1:ny)';

% Initialize ym -- predicted outputs due to inputs and filtering.

%     ym = [y1 y2 ... yny] has dimension Pnstep * ny.

    nstep = (nrow - ny - 2)/ny;

    Pnstep = max([z nstep]);

    ym = y0;

    for i = 2:Pnstep,

        ym = [ym;y0];

    end

% Initialize ymd -- predicted outputs due to measured disturbances.

%     ymd has the same structure as ym

    ymd = zeros(Pnstep,ny);

    dist = sysu(ny+1:ny+nd) - ud0(nu+1:nu+nd)';

% Call mpcsim to determine KF and check everything for consistency.

```

```

[dummy1,dummy2,dummy3,KF] =
mpcsim(model,model,Kmpc,0,r,usat,tfilter,dmodel,dmodel,[]);

[rKF,cKF] = size(KF);

if rKF == Pnstep*ny,

    KF(ny*Pnstep+1:ny*(Pnstep+1),:) = zeros(ny);

end

%

% Determine Ad (See the paper by Lee and Morari, 1993)

%

Ad = zeros(ny);

[nrf,ncf] = size(tfilter);

if nrf <= 1,

    for i = 1:ny,

        if (model(nrow-ny-1+i)==0)

            Ad(i,i)=1;

        else

            Ad(i,i)=0;

        end;

    end

else

    for i = 1:ny,

        if tfilter(2,i)==0

            Ad(i,i)=0;

        else

```

```

        Ad(i,i)= exp(-tsamp/tfilter(2,i));

    end;

end

end;

Xd = zeros(ny,1);

k = 0;

save tpm10217 ym ymd Xd k KF Ad dist

end

if abs(round(t/tsamp) - t/tsamp) < 1e-8,

    load tpm10217;

% Set up dSu and dSud

% If output i is integrating, then dSu(i,i) = 1; otherwise, dSu(i,i) = 0.

% Same for dSud

dSu = diag(1-model(nrow-ny-1:nrow-2,1));

if nd ~= 0,

    dSud = diag(1-dmodel(nrow-ny-1:nrow-2,1));

end

nstep = (nrow - ny - 2)/ny;

nstepd = (nrow - ny - 2)/ny;

Pnstep = max([z nstep nstepd]);

Su = model(1:nrow-ny-2,:);    % Step response coefficients

if Pnstep > nstep,            % Extend SR for plant model.

    Diffmod = model(nrow-2*ny-1:nrow-ny-2,:)-model(nrow-3*ny-1:nrow-2*ny-2,:);

    for i = 1:Pnstep-nstep,

```

```

    Su = [Su;model(nrow-2*ny-1:nrow-ny-2,:)+i*dSu*Diffmod];

end

end

if nd ~= 0,

    Sud = dmodel(1:nrow-ny-2,:); % Step response coefficients

    if Pnstep > nstepd, % Extend SR for disturbance model

        Diffmod = dmodel(nrow-2*ny-1:nrow-ny-2,:)-dmodel(nrow-3*ny-1:nrow-2*ny-
2,:);

        for i = 1:Pnstep-nstepd,

            Sud = [Sud;dmodel(nrow-2*ny-1:nrow-ny-2,:)+i*dSud*Diffmod];

        end

    end

% Calculate outputs due to measured disturbances

    distprev = dist; % Disturbance at previous sampling time

    dist = yp(ny+1:ny+nd)-ud0(nu+1:nu+nd); % Disturbance at current
sampling time

    ymd = [ymd(2:Pnstep,:); ymd(Pnstep,:)];

    ymd(Pnstep,:) = ymd(Pnstep,:) + (ymd(Pnstep,:) - ymd(Pnstep-1,:))*dSud;

    ymd = ymd + reshape(Sud*(dist-distprev),ny,Pnstep)';

end

%

% Update ym and Xd based on the current measurement, yp.

%

yerror = yp(1:ny) - ym(1,:) - ymd(1,:);

```

```
ym = ym + reshape(KF(1:ny*Pnstep,:)*yerror,ny,Pnstep)';
```

```
ym = [ym(2:Pnstep,:); ym(Pnstep,:)+(ym(Pnstep,:)-ym(Pnstep-1,:))*dSu + Xd'];
```

```
Xd = Ad*(Xd + KF(ny*Pnstep+1:ny*(Pnstep+1),:) * yerror);
```

```
%
```

```
% Create actual reference trajectory, r1, at sampling time k
```

```
%
```

```
if isempty(r),
```

```
    r = zeros(1,ny);
```

```
end
```

```
[N,ncolr]=size(r);
```

```
if N > Pnstep+k,
```

```
    r1 = r(k+1:Pnstep+k,:);
```

```
elseif N < k+2,
```

```
    r1 = r(N,:);
```

```
    for i = 1:Pnstep-1,
```

```
        r1 = [r1;r(N,:)];
```

```
    end
```

```
else
```

```
    r1 = r(k+1:N,:);
```

```
    for i = 1:Pnstep-N+k,
```

```
        r1 = [r1;r(N,:)];
```

```
    end
```

```
end
```

```
%
```


% Calculate fake reference trajectory, $r_f = r_1 - y_m$.

% Idea: $r(k+1) - y(k+1|k) = r(k+1) - M * y(k|k) - S \text{ delu}$

% $= r_1 - y_m - S \text{ delu} = r_f - S \text{ delu}$.

$r_f = r_1 - y_m - y_{md}$;

%

% Recompute the limits on the manipulated variables.

% $us_{at} = [u_{min1}(1) \dots u_{minnu}(1) u_{max1}(1) \dots u_{maxnu}(1) d_{max1}(1) \dots d_{maxnu}(1)]$

% $\dots \dots \dots$

% $[u_{min1}(N) \dots u_{minnu}(N) u_{max1}(N) \dots u_{maxnu}(N) d_{max1}(N) \dots d_{maxnu}(N)]$

if isempty(usat),

$[y_{dummy}, \text{delu}] = \text{mpcsim}(\text{model}, \text{model}, K_{mpc}, 0, r_f)$;

else

$[N, n_{colus_{at}}] = \text{size}(us_{at})$;

if $N > k$,

$us_{at1}(1:N-k, 2*nu+1:3*nu) = us_{at}(1:N-k, 2*nu+1:3*nu)$;

for $i = 1:nu$,

$us_{at1}(1:N-k, i) = us_{at}(k+1:N, i) - x(i)$;

$us_{at1}(1:N-k, nu+i) = us_{at}(k+1:N, nu+i) - x(i)$;

end

else,

$us_{at1}(N, 2*nu+1:3*nu) = us_{at}(N, 2*nu+1:3*nu)$;

for $i = 1:nu$,

$us_{at1}(1, i) = us_{at}(N, i) - x(i)$;

$us_{at1}(N, nu+i) = us_{at}(N, nu+i) - x(i)$;

end

end

%

% Determine the optimal control moves.

%

[ydummy,delu] = mpcsim(model,model,Kmpc,0,rf,usat1);

end

%

% Update ym based on delu. At this instant, $y_m = y(k+1|k)$.

%

$y_m = y_m + \text{reshape}(Su * \text{delu}', ny, Pnstep)';$

$sys = x + \text{delu}';$

$k = k + 1;$

save tpm10217 ym ymd Xd k KF Ad dist

end

else, % not interested

sys = [];

end

% End of function nlmpcsim.

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